NBS MONOGRAPH 25—SECTION 7

Standard X-ray Diffraction Powder Patterns

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

NATIONAL BUREAU OF STANDARDS

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.
[2] Located at Boulder, Colorado 80302.
[3] Located at 5285 Port Royal Road, Springfield, Virginia 22151.

UNITED STATES DEPARTMENT OF COMMERCE
Maurice H. Stans, *Secretary*
National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

H. E. Swanson, H. F. McMurdie, M. C. Morris,
and E. H. Evans

U.S. National Bureau of Standards Monograph 25—Section 7
Nat. Bur. Stand. (U.S.), Monogr. 25 Section 7, 188 pages (Sept. 1969)
CODEN: NBSMA

Issued September 1969

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402 - Price $1.50

Library of Congress Catalog Card Number: 53–61386

Contents

Errata

Monograph 25, Section 7

Monograph 25

Sec. 4, p. 4, column 2; at line 4 in the table, for *hkl* (211), the 2θ value for Tungsten (W) should be 73.184

Sec. 4, p. 23, *hkl's* for 2.036, 1.815, and 1.3505 should be $\bar{1}04$, $\bar{2}21$, and $\bar{4}01$ respectively.

Sec. 6, p. 4; in the 13th line from the end, the formula should be MgF_2

Sec. 6, p. 22; the space group symbol should be $C_3^6 v$ - R3c

Sec. 6, p. 42; the error for the NBS lattice constant in the table should be ±.0001

Sec. 6, p. 63; the second word of the title should be Magnesium

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Information on ten volumes in this series listed as follows is available from Mr. Howard E. Swanson, Room A221, Materials Building, National Bureau of Standards, Washington, D. C., 20234:

NBS Circular 539, Volume 1, Standard X-ray Diffraction Powder Patterns (Data for 54 substances).
NBS Circular 539, Volume 2, Standard X-ray Diffraction Powder Patterns (Data for 30 substances).
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NBS Circular 539, Volume 4, Standard X-ray Diffraction Powder Patterns (Data for 42 substances).
NBS Circular 539, Volume 5, Standard X-ray Diffraction Powder Patterns (Data for 45 substances).
NBS Circular 539, Volume 6, Standard X-ray Diffraction Powder Patterns (Data for 44 substances).
NBS Circular 539, Volume 7, Standard X-ray Diffraction Powder Patterns (Data for 53 substances).
NBS Circular 539, Volume 8, Standard X-ray Diffraction Powder Patterns (Data for 61 substances).
NBS Circular 539, Volume 9, Standard X-ray Diffraction Powder Patterns (Data for 43 substances).
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 7.—Data for 81 substances

Howard E. Swanson, Howard F. McMurdie,[1] Marlene C. Morris,[1] and Eloise H. Evans[1]

Standard x-ray diffraction powder patterns are presented for 81 substances. Forty-five of these patterns represent experimental data and 36 are calculated. The experimental x-ray powder diffraction patterns were obtained with a Geiger or proportional counter x-ray diffractometer, using samples of high purity. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings and from consideration of space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; peak intensities; reference intensities; lattice constants; powder patterns; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File [1968][2] is a compilation of diffraction patterns, gathered from many sources and produced under the auspices of the Joint Committee on Powder Diffraction Standards.[3] The File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, our program at the National Bureau of Standards contributes new data for this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 81 compounds (45 experimental and 36 calculated patterns), and is the seventeenth of the series of "Standard X-ray Diffraction Powder Patterns."[4]

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory. Treating the sample by appropriate annealing, recrystallizing, or heating in hydrothermal bombs improved the definition of most of the patterns. A check of phase purity was usually provided by the x-ray pattern itself, when it was indexed by comparison with computed d-values.

Optical data, color. A microscopic inspection for phase purity was made on the nonopaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, with oils standardized in sodium light, in the range 1.40 to 2.1.

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Structure, lattice constants. The space groups are listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography Vol. 1 [1952].

Orthorhombic cell dimensions are presented according to the Dana convention b>a>c [Palache et al., 1944].

A computer program [Evans et al., 1963] assigned *hkl's* and refined the lattice constants. Cell refinement was based only upon 2θ values which could be indexed without ambiguity. The number of significant figures reported for d-values varies slightly with the symmetry and crystallinity of each sample. Unit cell constants and their standard errors are based on least squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals.

Published unit cell data in kX units and data given in angstrom units prior to 1947 were converted to angstrom units using the factor 1.00206 reported by Bearden [1964].

Density. The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are computed using the Avogadro number (6.02252×10^{23}) and using atomic weights based on carbon 12 [International Union, 1961].

Interplanar spacings. Specimens for the interplanar spacing patterns were prepared by packing into a shallow holder a sample containing approximately 5 wt. percent tungsten powder that served as an internal standard. When tungsten lines were found to interfere, 25 percent silver was used in

[1] Research Associate, at the National Bureau of Standards, sponsored by the Joint Committee on Powder Diffraction Standards.

[2] Dates in brackets indicate the literature references at the end of each section of this paper.

[3] This committee is sponsored jointly by the American Society for Testing and Materials, the American Crystallographic Association, the (British) Institute of Physics, and The National Association of Corrosion Engineers.

[4] See previous page for listing of other published volumes.

place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid aberrations at the top of the peak, the reading for low values of 2θ was taken at a position about 25% of the way down from the top, and in the center of the peak width. For higher values of 2θ, where α_1 and α_2 peaks were resolved, the α_1 peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of 2θ. The internal standard lattice constants used were 3.16516 Å for tungsten and 4.08641 Å for silver at 25 °C, as determined by Swanson, Morris, and Evans [1966] and modified to correspond with the Bearden [1964] wavelength. (Prior to this, the internal standard constants used were 3.1648 Å and 4.0861 Å, through June 1966, and then 3.16504 Å and 4.08625 Å until June 1968.) All of the NBS patterns, unless otherwise noted, were made on a diffractometer at 25 °C using copper radiation with a monochromator having a curved lithium fluoride crystal. The wavelength of CuKα_1 was assumed to be 1.54056 Å [Bearden, 1964].

Intensity measurements. At least three patterns for intensity measurements were prepared for each sample to check reproducibility. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μ as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Fig. 1), and the powdered sample was drifted into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Fig 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line.

Reference intensity. For reference intensity measurements, αAl_2O_3 (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture is mounted in our regular intensity sample holder (illust. pg. 3). Only the portion of the x-ray pattern that includes the strongest line of each component is run; for the standard, the (*113*) reflection with d=2.085 Å is used. The direct ratio of the heights of the two lines is then reported as $I/I_{corundum}$. In a few instances the strongest line of one of the materials may fall on a line of the other. In this case, the second strongest line is measured, and based upon previous knowledge of the relative peak heights, a correction is made, thus enabling one to calculate the value for the strongest line.

CALCULATED POWDER PATTERNS

Since some substances are not readily available for experimental work, calculated powder patterns were made. These were based on published crystal structure data using a FORTRAN program developed by Smith [1967].

Lattice parameters. Before the computations of the patterns, corrections were made as necessary in the published lattice parameters so that they would correspond to the Bearden [1964] value of the copper wavelength; specifically, the published parameter in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, they were used directly from the International Tables [1962]. We have referred to this source by table number 3.3.1A or 3.3.1B, and 3.3.2A or 3.3.2B; they are found respectively on pages 202, 210, 213, and 214 of the International Tables, Vol. III [1962]. Corrections were made for dispersion if the authors had done so.

Thermal parameters. When these parameters were used directly as given by the authors, the reference is specified. When, for reasons necessitated by the computer program, the parameters were modified here, no reference is given.

Scale factors. For each compound, this conversion factor when multiplied by the scaled *integrated* intensities will reproduce the unscaled intensities derived from the structure factors for a single unit cell for the copper Kα_1 wavelength. The scale factors are not usable for comparisons between compounds since they have not been standardized for the effects of volume and absorption.

Integrated intensities. Intensity calculations were based on the copper Kα_1 wavelength, 1.54056 Å, determined by Bearden [1964]. The integrated intensities were computed from the formula:

$$I = F^2 \, (Lp) \, (FAC)$$

where F is the standard structure factor
FAC is the powder multiplicity

and $$Lp = \frac{1+2\cos^2 2\theta}{\sin^2 \theta \cos \theta}$$

The intensities are scaled to the strongest line as 100. Reflections with intensities equal to or less than 0.7 are not reported.

Peak intensities. In the Smith program, the integrated intensities can be assigned a Cauchy profile, and a half-width can be designated so as to simulate a trace from diffractometers in current use. The value of the half-width used here was 0.075° at 40° (2θ). The program then sums the intensities from the overlapping peak profiles and scales the resulting peak intensities to the strongest peak height. Reflections are not reported which had peak heights equal to or less than 0.7. When adjacent peaks have nearly equal 2θ values, resolution of individual peaks in the powder pattern would be unlikely; therefore, one composite peak is given. The angle of this peak is assigned the *hkl* of the reflection with the greatest integrated intensity.

The authors are indebted to J. H. deGroot for the preparation of many samples used, and to S. J. Carmel for his assistance with the work, particularly in performing intensity measurements.

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ISCC-NBS Centroid Color Charts, Standard Sample No. 2106, obtained from the Office of Standard Reference Materials, Room B328, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. $3.00 per set.

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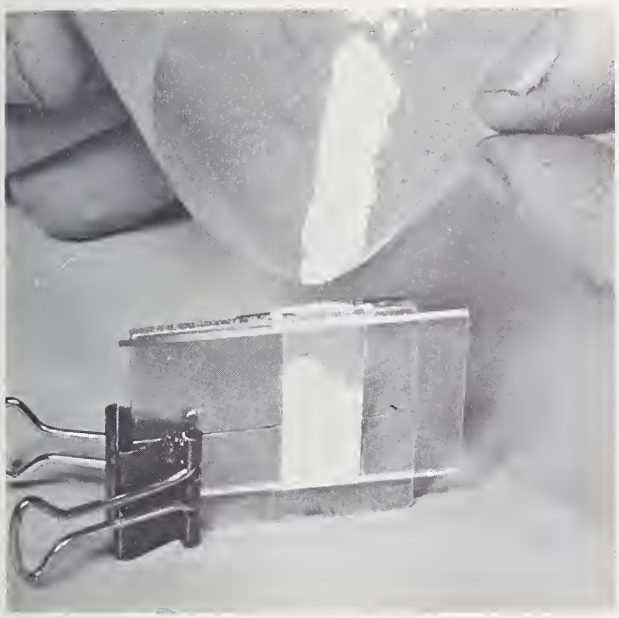

Figure 1

Figure 2

Sample

The sample was prepared at NBS by partial evaporation at 90° C of a water solution of $(NH_4)_2SO_4$ and $CdSO_4$, in a 2:1 weight ratio. The resulting double salt was washed with water and alcohol.

Major impurities

0.001-0.01% each: Ca, Mg, and Mn

Color

Colorless

Optical data

Isotropic, N=1.603

Structure

Cubic, $P2_13$ (198) Z=4, langbeinite type, [Gattow and Zemann,1958].

Lattice constants

	a(Å)
Jona and Pepinsky [1956]--------	10.35 ±.005
Gattow and Zemann [1958]--------	10.350 ±.003
NBS, sample at 25 °C----------	10.3511 ±.0001

Density

(calculated) 3.288 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

Polymorphism

Inverts below -186° C to a ferroelectric form [Jona and Pepinsky, 1956].

References

Gattow, G.and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Jona, F. and R. Pepinsky (1956). Ferroelectricity in the langbeinite system, Phy. Rev. 103, 1126.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.973	50	111	14.82
4.628	63	210	19.16
4.225	11	211	21.01
3.449	20	221	25.81
3.271	100	310	27.24
3.121	11	311	28.58
2.870	9	320	31.14
2.765	65	321	32.35
2.587	1	400	34.65
2.511	9	410	35.73
2.441	1	411	36.79
2.375	5	331	37.85
2.259	6	421	39.88
2.207	1	332	40.86
2.113	20	422	42.76
2.071	10	430	43.68
2.030	20	510	44.59
1.993	13	511	45.48
1.922	18	520	47.26
1.890	1	521	48.10
1.831	1	440	49.77
1.801	10	522	50.64
1.774	6	530	51.46
1.750	1	531	52.22
1.703	1	610	53.80
1.6788	17	611	54.62
1.6364	7	620	56.16
1.6166	8	621	56.91
1.5974	6	541	57.66
1.5786	2	533	58.41
1.5606	1	622	59.15
1.5433	3	630	59.88
1.5260	7	631	60.63
1.4938	2	444	62.08
1.4784	5	632	62.80
1.4640	5	710	63.49
1.4497	3	711	64.19
1.4360	1	640	64.88
1.4219	5	720	65.60
1.4086	3	721	66.30

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.3832	2	642	67.68
1.3709	2	722	68.37
1.3591	1	730	69.05
1.3478	1	731	69.71
1.3252	2	650	71.08
1.3144	2	732	71.75
1.2841	3	810	73.72
1.2742	2	811	74.39
1.2649	1	733	75.03
1.2556	1	820	75.68
1.2463	1	821	76.35
1.2374	1	653	77.00
1.2203	3	822	78.28
1.2114	1	830	78.96
1.2034	4	831	79.60
1.1952	3	751	80.25
1.1796	2	832	81.54
1.1721	2	752	82.17
1.1573	1	840	83.45
1.1502	1	841	84.09
1.1428	<1	910	84.76
1.1362	1	911	85.37
1.1294	1	842	86.00
1.1225	1	920	86.66
1.1160	3	921	87.29
1.1034	1	664	88.55
1.0971	4	922	89.19
1.0910	2	930	89.83
1.0849	1	931	90.47
1.0732	1	852	91.74
1.0676	1	932	92.36
1.0565	1	844	93.62
1.0509	<1	940	94.27
1.0455	2	941	94.91
1.0404	2	933	95.53
1.0298	3	10·1·0	96.83
1.0249	2	10·1·1	97.45
1.0150	<1	10·2·0	98.73
1.0101	1	10·2·1	99.38
1.0054	1	950	100.02
1.0006	1	951	100.67
0.9915	<1	10·3·0	101.95
.9869	1	10·3·1	102.61
.9739	1	10·3·2	104.55
.9694	1	871	105.24

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
.9654	<1	953	105.86
.9611	1	10·4·0	106.54
.9569	1	10·4·1	107.21
.9528	1	10·3·3	107.88
.9449	1	10·4·2	109.21
.9410	1	962	109.89
.9371	1	11·1·0	110.57
.9333	1	11·1·1	111.25
.9257	2	11·2·0	112.63
.9221	1	11·2·1	113.30
.9150	<1	880	114.67
.9113	2	11·2·2	115.40
.9078	1	11·3·0	116.11
.9042	1	11·3·1	116.83
.9009	1	10·4·4	117.53
.8976	1	964	118.23
.8943	2	11·3·2	118.94
.8876	1	10·6·0	120.41
.8844	1	11·4·0	121.14
.8813	<1	11·4·1	121.87
.8780	1	11·3·3	122.64
.8716	1	11·4·2	124.19
.8687	<1	965	124.92
.8626	1	12·0·0	126.49
.8596	2	12·1·0	127.29
.8567	2	12·1·1	128.09
.8538	2	11·5·1	128.90
.8480	2	12·2·1	130.55
.8451	1	11·5·2	131.41
.8395	1	12·2·2	133.13
.8369	2	12·3·0	133.97
.8341	1	12·3·1	134.87
.8315	1	11·5·3	135.76
.8261	1	12·3·2	137.64
.8235	2	11·6·1	138.59
.8183	1	12·4·0	140.53
.8158	2	12·4·1	141.54
.8133	1	12·3·3	142.58
.8108	1	991	143.62
.8083	<1	12·4·2	144.73
.8059	<1	10·8·1	145.82
.8034	2	11·6·3	146.98
.7986	1	10·8·2	149.38
.7963	1	12·5·0	150.65
.7939	1	13·1·0	152.00

Sample

Needle shaped crystals were obtained after partial evaporation of a solution of equimolar amounts NH_4Cl and $CuCl_2$ in anhydrous ethyl alcohol. X-ray patterns were produced from samples in a dry-air mounting to prevent hydration.

Major impurities

0.001-0.01% each: Ca, Cr, Fe, and Mg

0.1 -1.0 % each: Ni

Color

Moderate reddish brown

Optical data

Anisotropic, N_α=1.660, N_γ=1.850. Strongly pleochroic. Crystals were very fine.

Structure

Monoclinic, $P2_1/c$ (14) Z=4. Structure was determined by Willett et al.,[1963]

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
Willett et al.-[1963]	4.066 ±.005	14.189 ±.003	9.003 ±.004	97°30′ ± 5′
NBS sample at 25 °C	4.030 ±.001	14.187 ±.002	8.978 ±.002	96°28′ ± 1′

Density

(calculated) 2.447 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 0.6

References

Willett, R.D., C. Dwiggens Jr., R.F. Kruh, and R. E. Rundle (1963). Crystal structures of $KCuCl_3$ and NH_4CuCl_3, J. Chem. Phys. 38, 2429-2436.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.54	88	011	11.73
7.08	100	020	12.50
5.552	58	021	15.95
4.462	17	002	19.88
4.257	10	012	20.85
4.178	18	031	21.25
3.688	47	$\bar{1}11$	24.11
3.546	10	040	25.09
3.244	17	032	27.47
3.161	52	$\bar{1}02$	28.21
3.088	35	$\bar{1}12$	28.89
2.967	10	$\bar{1}31$	30.09
2.888	49	$\bar{1}22$	30.94
2.818	25	131	31.73
2.777	58	042	32.21
2.743	18	023	32.62
2.704	22	051	33.10
2.656	12	140	33.72
2.626	28	$\bar{1}32$,122	34.11
2.395	18	052	37.52
2.363	8	060	38.05
2.315	19	151	38.87
2.286	25	061	39.39
2.209	6	142	40.82
2.127	11	024	42.47
2.089	12	062	43.27
2.058	16	$\bar{1}43$	43.95
2.017	16	034	44.89
1.976	10	071	45.88
1.961	9	161	46.25
1.911	15	143	47.53
1.887	17	044,$\bar{1}53$	48.17
1.846	13	114,072	49.32
1.808	19	170	50.42
1.791	11	$\bar{1}71$	50.94
1.7739	11	$\bar{1}44$,080	51.47
1.7549	11	171,202	52.07
1.6746	5	073	54.77

Sample

The material was crystallized at 100 °C from an aqueous solution of stoichiometric amounts of $(NH_4)_2SO_4$ and $MnSO_4$.

Color

Colorless

Optical data

Isotropic, N=1.602

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type, [Gattow and Zemann, 1958]. The langbeinite structure was described by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]-------	10.192 ±.003
NBS, sample at 25 °C----------	10.1892 ±.0001

Density

(calculated) 2.726 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.4$

References

Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$ Acta Cryst. 10, 409-413.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.87	33	111	15.07
4.55	23	210	19.49
4.156	25	211	21.36
3.600	5	220	24.71
3.396	14	221	26.22
3.220	100	310	27.68
3.071	13	311	29.05
2.825	6	320	31.65
2.722	55	321	32.88
2.473	4	410	36.30
2.402	2	411	37.41
2.338	3	331	38.48
2.223	4	421	40.54
2.172	2	332	41.54
2.080	13	422	43.48
2.038	7	430	44.41
1.999	9	510	45.34
1.961	7	511	46.25
1.892	17	520	48.05
1.861	4	521	48.91
1.774	14	522	51.47
1.748	5	530	52.30
1.722	<1	531	53.15
1.699	<1	600	53.91
1.6749	3	610	54.76
1.6527	17	611	55.56
1.6109	5	620	57.13
1.5916	4	621	57.89
1.5728	3	541	58.65
1.5540	1	533	59.43
1.5362	<1	622	60.19
1.5193	7	630	60.93
1.5023	7	631	61.69
1.4711	2	444	63.15
1.4560	5	632	63.88
1.4413	4	710	64.61
1.4272	2	711	65.33
1.4128	2	640	66.08
1.3997	5	720	66.78
1.3866	4	721	67.49

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.3617	3	642	68.90
1.3498	2	722	69.59
1.3378	1	730	70.31
1.3266	4	731	70.99
1.3047	2	650	72.37
1.2942	2	732	73.05
1.2733	<1	800	74.45
1.2639	3	810	75.10
1.2544	2	811	75.77
1.2446	1	733	76.47
1.2356	1	820	77.13
1.2268	1	821	77.79
1.2180	1	653	78.46
1.2008	2	822	79.80
1.1926	1	830	80.46
1.1844	4	831	81.14
1.1765	3	751	81.80
1.1611	2	832	83.12
1.1536	2	752	83.78
1.1392	<1	840	85.09
1.1321	1	841	85.75
1.1250	<1	910	86.42
1.1184	1	911	87.06
1.1118	1	842	87.71
1.1053	1	920	88.36
1.0987	3	921	89.03
1.0860	1	664	90.35
1.0800	3	922	91.00
1.0740	3	930	91.65
1.0681	2	931	92.30
1.0567	1	852	93.60
1.0510	2	932	94.26
1.0399	1	844	95.59
1.0345	1	940	96.25
1.0293	2	941	96.90
1.0241	1	932	97.56
1.0189	1	10·0·0	98.23
1.0138	4	10·1·0	98.89
1.0089	2	10·1·1	99.55
0.9993	1	10·2·0	100.86

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
.9943	3	10·2·1	101.55
.9897	2	950	102.21
.9851	1	951	102.87
.9805	<1	10·2·2	103.55
.9760	2	10·3·0	104.23
.9714	2	10·3·1	104.92
.9585	2	10·3·2	106.95
.9544	2	871	107.63
.9503	2	953	108.31
.9460	1	10·4·0	109.02
.9420	2	960	109.72
.9380	1	10·3·3	110.41
.9302	1	10·4·2	111.80
.9264	1	962	112.50
.9224	1	11·1·0	113.25
.9188	<1	11·1·1	113.93
.9114	1	11·2·0	115.38
.9078	1	11·2·1	116.10
.9006	1	880	117.59
.8971	2	11·2·2	118.32
.8938	1	11·3·0	119.05
.8902	<1	11·3·1	119.82
.8868	1	10·4·4	120.59
.8835	2	964	121.35
.8802	3	11·3·2	122.11
.8737	1	10·6·0	123.68
.8705	1	11·4·0	124.48
.8673	2	11·4·1	125.28
.8642	2	11·3·3	126.09
.8581	1	11·4·2	127.71
.8550	1	965	128.55
.8491	1	12·0·0	130.24

Sample

The sample was prepared at NBS by E. Levin. Stoichiometric amounts of barium nitrate and boric acid were ground together and heated near 800°C.

Color

Colorless

Optical data

Biaxial (-) N_α=1.558, N_γ=1.590, 2V is small.

Structure

Orthorhombic, Z=8 [Krogh-Moe, 1960].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
Krogh-Moe[1960]--	8.56	17.38	13.20
NBS, sample at 25°C--	8.550 ±.001	17.352 ±.002	13.211 ±.003

Density

(calculated) 2.927 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.4

Polymorphism

A high temperature tetragonal form is being studied by Levin and Robbins [private communication]

Additional patterns

1. PDF card 6-0277 [McMurdie and Levin, 1949].

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
7.25	10	021	12.20
6.09	55	120	14.54
5.24	100	102	16.92
4.35	6	032,040	20.42
4.277	5	200,013	20.75
4.120	13	041	21.55
4.068	8	201	21.83
3.916	6	103	22.69
3.872	13	132,140	22.95
3.836	6	220	23.17
3.714	13	141	23.94
3.682	5	221	24.15
3.625	5	042	24.54
3.590	7	202	24.78
3.572	9	123	24.91
3.515	2	212	25.32
3.337	95	142	26.69
3.316	100	222	26.86
3.124	3	151	28.55
3.081	14	104	28.96
3.047	30	232,240	29.29
2.965	2	241	30.12
2.904	} 80 {	124	30.77
2.895		060,223	30.86
2.826	4	061	31.64
2.740	25	160	32.65
2.709	25	233,320	33.04
2.683	11	161	33.37
2.650	16	321,062	33.80
2.617	25	302	34.24
2.531	5	162	35.43
2.524	6	105	35.54
2.510	7	144,331	35.75
2.502	9	243,224	35.86
2.418	5	063	37.15
2.393	4	303,054	37.56
2.380	3	234,170,+	37.76
2.346	3	341,171	38.34
2.326	4	163	38.68
2.306	4	323	39.02

Internal standard Ag, a = 4.08641 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.251	30	262	40.02
2.241	50	342,172	40.20
2.238		244	40.27
2.169	14	080	41.60
2.138	20	400	42.23
2.132	25	026,106	42.35
2.122	8	410	42.56
2.111	11	401,164	42.81
2.105	17	263,180,+	42.93
2.094	19	173,324,+	43.17
2.076	7	181,420	43.57
2.050	6	421	44.13
2.033	3	402	44.52
2.003	10	182,136	45.24
1.980	12	422	45.79
1.945	5	083,216	46.67
1.938	6	264,305	46.83
1.935	7	280	46.91
1.922	5	403	47.25
1.918	7	432,440	47.37
1.913	11	281,146,+	47.48
1.907	13	091	47.64
1.898	6	441,183	47.88
1.878	2	423,017	48.43
1.856	3	282	49.04
1.841	2	442	49.46
1.813	3	084	50.28
1.794	4	404,037	50.85
1.774	5	265,184	51.46
1.769	5	345,175	51.61
1.741	5	306,291	52.51
1.729	6	193,364	52.92
1.719	3	460,217	53.25
1.712	3	381	53.49
1.702	3	510,1·10·0	53.83
1.687	5	511,1·10·1	54.34
1.679	7	0·10·2,520	54.61
1.670	6	382,284,+	54.95
1.665	9	094,275,+	55.11
1.657	7	502	55.42

References

Krogh-Moe, J. (1960). A note on the structure of barium tetraborate, Acta Chem. Scand. 14, No. 5, 1229-1230.

Levin, E.M. and H.F. McMurdie (1949). The system $BaO-B_2O_3$, J. Res. Natl. Bur. Std. 42, (RP1956) 131-138.

Sample

The sample was prepared by melting a stoichiometric mixture of Cs_2SO_4 and $CaSO_4$ followed by annealing for 18 hours at 700 °C.

Color

Colorless

Optical data

Isotropic, N=1.549

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann,1958]. The langbeinite structure was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]--------	10.724 ±.005
NBS, sample at 25 °C----------	10.7213 ±.0001

Density

(calculated) 3.417 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.8$

References

Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-typ, $A_2^+B_2^{2+}(SO_4)_3$, Z.Anorg. Allgem. Chem. 293, 233-240.

Zemann, A. and J. Zemann (1957). Die Kristallstructur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Internal standard Ag, a = 4.08641 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.18	16	111	14.32
4.79	9	210	18.51
4.373	7	211	20.29
3.792	12	220	23.44
3.574	8	221	24.89
3.391	100	310	26.26
3.234	18	311	27.56
3.095	1	222	28.82
2.973	21	320	30.03
2.865	53	321	31.19
2.599	23	410	34.48
2.525	1	411	35.52
2.460	8	331	36.50
2.397	3	420	37.49
2.339	7	421	38.45
2.286	9	332	39.38
2.188	16	422	41.22
2.145	2	430	42.10
2.102	30	510	43.00
2.063	2	511	43.84
1.991	8	520	45.52
1.958	2	521	46.33
1.897	<1	440	47.92
1.866	4	522	48.75
1.839	1	530	49.52
1.812	2	531	50.30
1.788	1	600	51.05
1.762	4	610	51.84
1.739	17	611	52.59
1.695	6	620	54.05
1.675	9	621	54.77
1.654	8	541	55.50
1.635	2	533	56.23
1.617	1	622	56.89
1.598	7	630	57.64
1.5806	5	631	58.33
1.5471	4	444	59.72
1.5318	2	632	60.38
1.5163	1	550	61.06
1.5010	1	711	61.75
1.4867	1	640	62.41
1.4723	2	720	63.09
1.4589	6	721	63.74
1.4328	4	642	65.04
1.4208	1	722	65.66

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
1.4079	3	730	66.34
1.3958	3	731	66.99
1.3729	2	650	68.26
1.3612	3	732	68.93
1.3403	1	800	70.16
1.3299	2	810	70.79
1.3198	1	811	71.41
1.3097	1	733	72.05
1.3002	1	820	72.66
1.2909	4	821	73.27
1.2814	2	653	73.90
1.2636	2	822	75.12
1.2548	1	830	75.74
1.2464	5	831	76.34
1.2382	2	751	76.94
1.2220	<1	832	78.15
1.2139	2	752	78.77
1.1913	1	841	80.57
1.1838	1	910	81.19
1.1767	2	911	81.78
1.1696	1	842	82.38
1.1628	1	920	82.97
1.1560	3	921	83.57
1.1431	1	664	84.73
1.1365	3	922	85.34
1.1302	3	930	85.93
1.1241	<1	931	86.51
1.1119	1	852	87.70
1.1059	2	932	88.30
1.0886	1	940	90.08
1.0831	1	941	90.66
1.0778	1	933	91.23
1.0722	1	10·0·0	91.85
1.0668	1	10·1·0	92.45
1.0618	<1	10·1·1	93.01
1.0514	1	10·2·0	94.21
1.0464	2	10·2·1	94.81
1.0415	2	950	95.39
1.0365	1	951	96.00
1.0317	1	10·2·2	96.59
1.0270	1	10·3·0	97.19
1.0221	2	10·3·1	97.81
1.0086	1	10·3·2	99.59
1.0041	<1	871	100.19
0.9998	<1	953	100.79

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
.9955	1	10·4·0	101.39
.9912	1	960	102.00
.9871	1	10·3·3	102.59
.9788	1	10·4·2	103.81
.9746	1	962	104.44
.9707	2	11·1·0	105.04
.9669	1	11·1·1	105.63
.9590	1	11·2·0	106.88
.9551	2	11·2·1	107.51
.9475	<1	880	108.78
.9439	1	11·2·2	109.38
.9368	1	11·3·1	110.62
.9332	1	10·4·4	111.26
.9296	<1	964	111.91
.9262	2	11·3·2	112.54
.9192	1	10·6·0	113.85
.9159	1	11·4·0	114.49
.9127	1	11·4·1	115.12
.9029	1	11·4·2	117.11
.8998	1	965	117.76
.8934	<1	12·0·0	119.12
.8904	1	12·1·0	119.79
.8873	1	12·1·1	120.47
.8844	1	11·5·1	121.15
.8814	<1	12·2·0	121.84
.8782	2	12·2·1	122.58
.8754	2	11·5·2	123.27
.8696	1	12·2·2	124.70
.8668	1	12·3·0	125.41
.8639	1	12·3·1	126.17
.8612	1	11·5·3	126.86
.8556	<1	12·3·2	128.40
.8529	1	11·6·1	129.15
.8475	1	12·4·0	130.70
.8449	1	12·4·1	131.48
.8423	1	12·3·3	132.25
.8398	1	991	133.04
.8371	1	12·4·2	133.89
.8347	<1	10·8·1	134.70
.8321	2	11·6·3	135.54

Sample

The material was made by slow evaporation at room temperature of an equimolar solution of $Cs_2(SO_4)$ and $CuSO_4$.

Color

Unground: brilliant greenish blue
Ground: very pale greenish blue

Optical data

Biaxial (+) N_α=1.504, N_β=1.506, N_γ=1.514
2V is medium

Structure

Monoclinic, $P2_1/a$ (14), Z=2.
$Cs_2Cu(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C----	9.439 ±.001	12.762 ±.002	6.310 ±.001	106°11′ ±1′

Density

(calculated) 2.864 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.2

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.37	11	110	11.98
6.06	4	001	14.60
5.47	4	$\bar{1}11$	16.18
5.21	8	120	16.99
4.54	6	200	19.55
4.39	13	021	20.19
4.31	40	$\bar{1}21$	20.61
4.25	100	$\bar{2}01$,111	20.90
4.026	14	$\bar{2}11$	22.06
3.852	60	130	23.07
3.696	5	220	24.06
3.439	8	$\bar{1}31$	25.89
3.227	25	201	27.62
3.192	25	040	27.93
3.126	16	211	28.53
3.089	25	$\bar{1}31$	28.88
3.030	25	$\bar{1}12$	29.16
3.027	4	002	29.48
2.984	12	$\bar{3}11$	29.92
2.948	20	012	30.29
2.939	20	310	30.39
2.926	25	$\bar{2}02$	30.53
2.878	15	221	31.05
2.825	25	$\bar{1}22$,041	31.65
2.799	9	$\bar{1}41$	31.95
2.765	10	$\bar{3}21$	32.35
2.732	9	320	32.75
2.658	5	$\bar{2}22$	33.69
2.609	3	240	34.35
2.603	4	112,141	34.43
2.569	6	231	34.90
2.553	6	$\bar{2}41$	35.16
2.531	10	$\bar{1}32$	35.43
2.488	25	$\bar{3}31$	36.07
2.456	13	150,122	36.56
2.403	2	311	37.40
2.348	17	$\bar{4}01$	38.30
2.311	5	$\bar{4}11$	38.94
2.284	12	321	39.41
2.266	20	241,400	39.74

Internal standard Ag, a = 4.08641 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.247	8	202	40.10
2.225	8	250	40.54
2.198	9	042	41.03
2.187	12	$\bar{2}51$	41.25
2.156	11	$\bar{2}42$	41.87
2.135	10	420	42.30
2.129	5	060	42.43
2.092	5	$\bar{4}12$	43.21
2.072	6	$\bar{2}03,\bar{1}13,+$	43.65
2.055	4	$\bar{4}31$	44.02
2.020	6	003	44.84
2.014	3	$\bar{4}22$	44.97
2.002	5	251,430	45.26
1.996	6	013,$\bar{1}23$	45.39
1.961	4	$\bar{3}51$	46.25
1.951	12	$\bar{4}01,350$	46.50
1.927	6	$\bar{3}13,023,+$	47.13
1.898	4	$\bar{4}32$	47.89
1.882	8	$\bar{1}33$	48.32
1.871	5	312	48.63
1.865	7	$\bar{3}23,\bar{2}33$	48.80
1.847	9	440	49.30
1.842	5	152	49.44
1.813	3	322	50.27
1.809	6	$\bar{5}21$	50.41
1.789	10	123,$\bar{1}70$	51.02
1.775	5	261,$\bar{5}12$	51.44
1.763	5	$\bar{1}62$	51.80
1.7562	5	$\bar{4}13$	52.03
1.7281	9	$\bar{4}51,332$	52.94
1.7072	6	133,043	53.64
1.6890	9	$\bar{1}71$	54.26
1.6634	5	$\bar{3}43$	55.17
1.6505	4	$\bar{5}32$	55.64
1.6362	3	$\bar{4}33$	56.17
1.6308	4	$\bar{4}52$	56.37
1.6090	6	143,$\bar{2}53$	57.20

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Sample

The sample was made by slow evaporation at room temperature of an equimolar solution of Cs_2SO_4 and $FeSO_4$.

Color

Unground: very pale green
Ground: colorless

Optical data

Biaxial(+) N_α=1.501, N_β=1.504, N_γ=1.516. 2V is medium

Structure

Monoclinic, $P2_1/a$ (14), Z=2, Isostructural with other "Tutton Salts" [Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	9.355 ±.001	12.893 ±.002	6.378 ±.001	106°53′ ±1′

Density

(calculated) 2.805 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.8

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.34	12	110	12.04
6.10	5	001	14.52
5.518	3	011	16.05
5.233	12	120	16.93
4.478	5	200	19.81
4.438	11	021	19.99
4.356	19	$\bar{1}21$	20.37
4.247	100	$\bar{2}01$	20.90
4.227		210,111	21.00
4.033	6	$\bar{2}11$	22.02
3.877	75	130	22.92
3.681	4	220,121	24.16
3.475	10	$\bar{1}31$	25.61
3.221	30	040	27.67
3.194	20	201	27.91
3.101	70	211,230,+	28.77
3.091		$\bar{1}12$	28.86
3.033	2	140	29.43
2.970	25	$\bar{3}11$,012	30.06
2.954	19	$\bar{2}02$	30.23
2.907	13	310	30.73
2.860	30	221	31.25
2.851		041	31.35
2.830	6	$\bar{1}41$	31.59
2.761	2	$\bar{3}21$,022	32.40
2.707	6	$\bar{3}20$	33.07
2.683	3	$\bar{2}22$	33.37
2.614	6	240,141	34.27
2.567	17	$\bar{2}41$	34.93
2.557	17	$\bar{1}32$	35.06
2.489	35	$\bar{3}31$,032	36.06
2.461	9	122	36.48
2.453	8	330	36.61
2.374	12	051	37.87
2.358	8	$\bar{3}22$	38.14
2.330	2	$\bar{4}01$	38.61
2.296	7	$\bar{4}11$	39.21
2.267	20	241,$\bar{1}42$	39.73
2.264	17	321,132	39.79
2.235	14	250,151	40.32

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.215	5	$\bar{3}41,042$	40.69
2.204	9	$21\bar{2},\bar{2}51,+$	40.92
2.176	13	$\bar{2}42$	41.47
2.149	3	060	42.02
2.114	8	420,222	42.74
2.094	6	$\bar{4}12,\bar{1}13,+$	43.16
2.050	3	$\bar{4}31$	44.14
2.035	7	003	44.48
2.017	3	$\bar{4}22,\bar{1}23$	44.91
2.006	6	251	45.16
1.992	2	$\bar{2}23,\bar{3}42$	45.50
1.970	12	$\bar{3}51,052$	46.04
1.946	6	$\bar{3}13$	46.64
1.918	6	$\bar{2}61$	47.36
1.903	8	$\bar{4}32,\bar{1}33$	47.75
1.882	5	$\bar{2}33,\bar{3}23$	48.32
1.853	3	$152,\bar{5}11$	49.14
1.838	11	440,242	49.56
1.803	5	170,322	50.57
1.796	10	$\bar{5}21,123$	50.78
1.785	4	$\bar{4}03$	51.13
1.781	5	$\bar{1}62$	51.25
1.773	6	$510,\bar{4}42,+$	51.50
1.759	3	$431,\bar{1}71$	51.93
1.725	5	520	53.05
1.721	9	$332,\bar{4}23,+$	53.17
1.703	8	270,171	53.78
1.664	2	213	55.15
1.650	7	$\bar{5}32$	55.65
1.638	2	$\bar{3}62,\bar{1}53$	56.11
1.626	2	$\bar{2}53$	56.56
1.606	1	$\bar{3}61$	57.32

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$, J.Chem. Soc. 63, 337-423.

Sample

The sample was made by slow evaporation at room temperature of an equimolar solution of Cs_2SO_4 and $MgSO_4$.

Color

Colorless

Optical data

Biaxial (+) N_α=1.481, N_β=1.485, N_γ=1.492
2V is medium.

Structure

Monoclinic, $P2_1/a$ (14), Z=2.
$Cs_2Mg(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	9.330 ±.001	12.848 ±.003	6.360 ±.001	107°2′ ±1′

Density

(calculated) 2.689 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.8

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.31	45	110	12.09
6.42	5	020	13.78
6.08	15	001	14.55
5.50	6	011	16.11
5.21	19	120	16.99
4.42	10	021	20.09
4.34	31	$\bar{1}21$	20.44
4.23	100	$\bar{2}01$	20.98
4.026	8	$\bar{2}11$	22.06
3.860	83	130	23.02
3.537	4	$\bar{2}21$	25.16
3.463	9	$\bar{1}31$	25.70
3.210	46	040	27.77
3.181	36	201	28.03
3.087	97	131,211	28.90
3.041	7	002	29.35
3.010	5	$\bar{2}31$	29.65
2.965	39	$\bar{3}11$	30.12
2.948	38	$\bar{2}02$	30.29
2.899	11	310	30.82
2.846	38	$\bar{1}22$	31.41
2.822	10	$\bar{1}41$	31.68
2.753	3	$\bar{3}21$	32.50
2.699	8	320	33.16
2.607	6	240,141	34.37
2.559	29	$\bar{2}41$	35.03
2.553	31	231	35.12
2.485	33	$\bar{3}31,\bar{3}12$	36.12
2.450	16	122	36.66
2.443	18	330	36.75
2.367	13	051,311	37.98
2.352	10	$\bar{3}22$	38.23
2.289	9	$\bar{4}11$	39.33
2.259	22	241,$\bar{1}42$	39.88
2.230	17	400	40.42
2.197	11	410,$\bar{2}51$	41.04
2.172	13	$\bar{2}42$	41.55
2.107	6	420	42.88
2.092	6	$\bar{2}03,\bar{4}12$	43.22
2.086	7	$\bar{1}13$	43.33

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.063	1	$\bar{2}13$	43.83
2.046	5	142,$\bar{4}31$	44.24
2.027	8	003	44.67
1.998	7	$\bar{1}52$,251	45.35
1.963	10	$\bar{3}51$,052	46.21
1.943	6	350	46.71
1.912	6	$\bar{2}61$	47.51
1.879	5	$\bar{2}33$,$\bar{3}23$	48.39
1.8326	12	033,440	49.71
1.7918	12	$\bar{5}21$	50.92
1.7886	11	123	51.02
1.7847	11	$\bar{3}33$	51.14
1.7689	7	$\bar{4}42$,510	51.63
1.7382	2	360	52.61
1.7203	6	520,$\bar{5}22$	53.20
1.7143	7	043,332	53.40
1.6970	6	270,171	53.99
1.6480	8	441,530	55.73
1.6354	3	$\bar{4}52$,$\bar{3}62$	56.20
1.6213	3	$\bar{2}53$	56.73

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Sample

The sample was made by slow evaporation at room temperature of an equimolar solution of Cs_2SO_4 and $MnSO_4$.

Color

Unground: purplish white
Ground: colorless

Optical data

Biaxial (+) N_α=1.495, N_β=1.497, N_γ=1.502
2V is large

Structure

Monoclinic, $P2_1/a$ (14), Z=2 Isostructural with other "Tutton Salts" [Tutton, 1893] The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25 °C	9.425 ±.001	12.976 ±.002	6.389 ±.001	107°10′ ±1′

Density

(calculated) 2.763 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.2

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.41	17	110	11.94
6.11	7	001	14.48
5.524	4	011	16.03
5.273	15	120	16.80
4.510	5	200	19.67
4.442	11	021	19.97
4.384	22	$\bar{1}21$	20.24
4.281	100	$\bar{2}01$	20.73
4.261	59	210	20.83
4.241	61	111	20.93
4.064	5	$\bar{2}11$	21.85
3.899	76	130	22.79
3.693	3	220	24.08
3.497	10	$\bar{1}31$	25.45
3.244	33	040	27.47
3.201	23	201	27.85
3.111	72	131, 211	28.67
3.103		$\bar{1}12$	28.75
3.049	3	002, 140	29.27
2.993	20	311	29.83
2.965	29	$\bar{2}02$	30.12
2.927	15	310	30.52
2.894	1	$\bar{2}12$	30.87
2.869	42	221	31.15
2.861	11	041, $\bar{1}22$	31.24
2.778	2	$\bar{3}21$	32.19
2.723	6	320	32.86
2.699	5	$\bar{2}22$	33.17
2.632	7	240	34.04
2.624	3	141	34.14
2.583	15	$\bar{2}41$	34.70
2.568	17	$\bar{1}32$	34.91
2.507	41	$\bar{3}31$	35.79
2.501	30	$\bar{3}12$	35.88
2.464	14	330, 122	36.44
2.388	12	051	37.63
2.374	9	$\bar{3}22$	37.87
2.349	2	$\bar{4}01$	38.28
2.311	11	$\bar{4}11$	38.94
2.277	22	241	39.54

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.271	20	321	39.65
2.250	12	400	40.04
2.239	11	202	40.25
2.232	3	$\bar{3}41$	40.38
2.218	13	410,$\bar{2}51$	40.64
2.187	15	$\bar{2}42$	41.24
2.162	2	060	41.74
2.127	8	420	42.47
2.110	6	$\bar{4}12$	42.82
2.103	7	160,$\bar{2}03$	42.98
2.075	2	$\bar{2}13$	43.59
2.065	3	$\bar{4}31$	43.81
2.035	10	003	44.49
2.016	7	251	44.93
2.005	6	$\bar{3}42$	45.19
1.984	6	$\bar{3}51$	45.69
1.977	12	052	45.86
1.953	8	$\bar{3}13$,$\bar{2}52$	46.45
1.929	7	$\bar{2}61$	47.08
1.907	10	$\bar{1}33$	47.66
1.891	5	$\bar{3}23$,$\bar{2}33$	48.07
1.866	3	$\bar{5}11$	48.75
1.849	11	113,440	49.24
1.843	6	242,033	49.40
1.817	3	$\bar{3}52$	50.16
1.810	8	$\bar{5}21$	50.37
1.796	11	123,$\bar{4}03$	50.78
1.783	8	$\bar{5}12$,510	51.19
1.771	3	351	51.57
1.740	2	$\bar{4}51$	52.55
1.735	5	$\bar{5}22$,520	52.72
1.730	5	$\bar{4}23$	52.87
1.725	6	332,043	53.06
1.712	9	171	53.49

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. **117**, 334-357.

Tutton, A.E.(1893). Connection between the atomic weight of contained metals and the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$ J. Chem. Soc. 63, 337-423.

Sample

The sample was prepared by mixing saturated solutions of $HgCl_2$ and CsCl at room temperature.

Color

Colorless

Optical data

Very low birefringence, N≅1.790

Structure

$CsHgCl_3$ has been reported as cubic [Natta and Passerini, 1928]. Náray-Szabó [1947], found it to be monoclinic with a=b=c and β~90°. In this work it is considered as a distorted perovskite and has been tentatively indexed as orthorhombic, isostructural with $NaMnF_3$ and $RbCaCl_3$. Very weak lines at 26.82, 27.94 and 29.50 °(2θ) suggest that a small amount of a second phase may be present, or that the material has a larger supercell. The assumed space group is Pnma (62) with Z equal to 4.

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
Natta and Passerini [1928][1]	5.45*		
Náray-Szabó [1947][2]	10.92*	10.92*	10.92*
NBS, sample at 25° C	7.688 ±.002	10.878 ±.002	7.669 ±.001

*from kX
[1] indexed as cubic
[2] indexed as monoclinic with β~90°.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.42	15	101	16.34
3.834	100	002	23.18
3.132	1	022	28.47
2.715	45	202	32.96
2.428	11	301,222,+	37.00
2.217	45	042,123	40.67
1.920	25	242	47.30
1.894	1	250,410	48.00
1.810	5	303,143,+	50.38
1.717	25	402,323,+	
1.570	6	440	58.75
1.567	6	044	58.90
1.506	2	501,343	61.51
1.453	15	442,521,+	64.03
1.451	17	244	64.14
1.357	3	404	69.16
1.319	2	460,181	71.45
1.317	2	064,424	71.59
1.279	5	325	74.05
1.214	6	444	78.74
1.187	1	381	80.94
1.184	1	226	81.16
1.159	2	640,561,+	83.27
1.157	2	046	83.50
1.110	3	480,642	87.89
1.108	3	264	88.10
1.087	1	464	90.30
1.065	5	604	92.59
1.064	4	406	92.73
1.010	1	662,741,+	99.43
1.008	1	266	99.65
.9921	2	644,723	101.86
.9911	2	446	102.01

Density

(calculated) 4.555 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.0$

References

Natta, G. and L. Passerini (1928). Isomorfismo, polimorfismo e morfotropia I.Composti del tipo ABX_3. Gazz.Chim.Ital. **58**, 472-484.

Náray-Szabó, S. (1947). The perovskite structure family, Müegyetemi, Kozlemen. No. 1, 30-41.

Sample

The sample was prepared by slow evaporation at room temperature of an equimolar solution of Cs_2SO_4 and $NiSO_4$.

Color

Unground: strong bluish green
Ground: very pale green

Optical data

Biaxial (-) N_α=1.507, N_β=1.512, N_γ=1.516
2V is very large

Structure

Monoclinic, $P2_1/a$ (14), Z=2.
$Cs_2Ni(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25°C----	9.264 ±.001	12.773 ±.002	6.359 ±.001	106°59′ ±1′

Density

(calculated) 2.883 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.7

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.284	10	110	12.14
6.083	6	001	14.55
5.487	6	011	16.14
5.184	12	120	17.09
4.405	12	021	20.14
4.327	18	$\bar{1}21$	20.51
4.215	100	$\bar{2}01$	21.06
4.201		111	21.13
4.001	6	$\bar{2}11$	22.20
3.837	70	130	23.16
3.641	4	220	24.43
3.448	10	$\bar{1}31$	25.82
3.193	25	040	27.92
3.168	20	201	28.14
3.074	70	131,211,+	29.02
3.005	2	140	29.71
2.961	12	012	30.16
2.943	30	$\bar{3}11,\bar{2}02$	30.35
2.877	14	310	31.06
2.839	30	221	31.49
2.806	7	$\bar{1}41$	31.87
2.738	1	$\bar{3}21$	32.68
2.681	8	320	33.40
2.673	6	$\bar{2}22$	33.50
2.591	6	112,240,+	34.59
2.545	25	$\bar{1}32,\bar{2}41,+$	35.24
2.468	30	$\bar{3}12,\bar{3}31$	36.37
2.447	11	122	36.69
2.428	4	330	37.00
2.354	12	051,311	38.20
2.342	10	$\bar{1}51,\bar{3}22$	38.41
2.310	2	$\bar{4}01$	38.96
2.272	9	$\bar{4}11$	39.64
2.249	20	132,241	40.06
2.243	20	321	40.17
2.222	7	202	40.57
2.213	13	151,250,+	40.73
2.201	5	042	40.97
2.184	9	$\bar{2}51$,410	41.30
2.163	13	$\bar{2}42$	41.73

Internal standard Ag, a = 4.08641 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.130	2	060	42.41
2.106	2	$\bar{4}02$	42.91
2.093	9	420	43.19
2.079	6	$\bar{4}12$	43.49
2.070	4	160	43.69
2.062	2	$\bar{2}13$	43.86
2.029	10	$\bar{4}31$,003	44.63
2.007	4	061,$\bar{1}23$	45.14
2.001	6	$\bar{1}61$,$\bar{4}22$	45.29
1.989	4	251	45.58
1.977	3	$\bar{3}42$	45.87
1.955	12	052	46.42
1.952	12	$\bar{3}51$	46.49
1.937	7	$\bar{3}13$	46.87
1.916	2	341	47.40
1.910	3	401	47.58
1.898	8	$\bar{2}61$	47.89
1.894	11	$\bar{1}33$	48.00
1.873	6	$\bar{3}23$	48.56
1.839	1	152	49.53
1.830	4	033,421	49.79
1.819	10	440	50.10
1.787	12	$\bar{1}70$,123	51.07
1.767	5	$\bar{1}62$,261	51.69
1.755	6	510	52.08
1.743	5	171,431,+	52.47
1.728	1	360	52.96
1.710	6	043,$\bar{4}23$	53.53
1.707	12	520,332	53.65
1.688	8	171,270	54.31
1.659	2	162	55.32
1.654	2	213	55.50
1.636	6	$\bar{5}32$,530	56.16
1.625	3	$\bar{3}62$,$\bar{4}52$	56.58
1.616	4	$\bar{2}53$	56.92
1.591	4	361	57.92
1.587	3	053,$\bar{2}04$	58.06
1.582	3	$\bar{1}72$,271	58.27
1.571	4	180,$\bar{5}13$,+	58.74
1.563	3	$\bar{3}71$	59.04
1.552	7	370,$\bar{4}43$	59.52

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Sample

The sample was prepared by slow evaporation at room temperature of an equimolar solution of Cs_2SO_4 and $ZnSO_4$.

Color

Colorless

Optical data

Biaxial (-) N_α=1.594, N_β=1.610, N_γ=1.615
2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2.
$Cs_2Zn(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	9.316 ±.001	12.815 ±002	6.373 ±.001	106°57′ ±1′

Density

(calculated) 2.881 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.3

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.31	8	110	12.10
6.095	3	001	14.52
5.504	3	011	16.09
5.202	9	120	17.03
4.451	7	200	19.93
4.416	10	021	20.09
4.337	16	$\bar{1}21$	20.46
4.227	100	$\bar{2}01$	21.00
4.019	5	$\bar{2}11$	22.10
3.854	60	130	23.06
3.660	4	121,220	24.30
3.461	9	$\bar{1}31$	25.72
3.204	25	040	27.82
3.185	15	201	27.99
3.087	65	131,$\bar{1}12$,+	28.90
2.962	20	$\bar{3}11$	30.15
2.951	20	$\bar{2}02$	30.26
2.896	11	310	30.85
2.850	30	$\bar{1}22$,221	31.36
2.816	6	$\bar{1}41$	31.75
2.749	2	$\bar{3}21$,022	32.54
2.695	5	320	33.21
2.678	4	$\bar{2}22$	33.43
2.601	6	240,112,+	34.45
2.552	18	231,$\bar{1}32$	35.13
2.479	30	$\bar{3}31$,$\bar{3}12$	36.21
2.452	8	122	36.62
2.439	4	330	36.82
2.362	9	051	38.07
2.351	8	$\bar{3}22$,$\bar{1}51$	38.25
2.321	2	$\bar{4}01$	38.76
2.284	7	$\bar{4}11$	39.41
2.256	19	132,$\bar{1}42$,+	39.92
2.229	8	400	40.43
2.222	9	151,250	40.56
2.209	4	042	40.81
2.194	7	410,$\bar{2}51$	41.11
2.170	11	$\bar{2}42$	41.59
2.135	2	060	42.30
2.105	8	420	42.94

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.092	4	$\bar{1}13$	43.22
2.088	3	$\bar{4}12$	43.30
2.040	3	$\bar{4}31$	44.37
2.032	7	003	44.55
2.009	3	$\bar{4}22,\bar{1}61$	45.09
1.996	3	$251,\bar{1}52$	45.39
1.978	1	232	45.83
1.962	8	052	46.24
1.941	6	350	46.75
1.907	5	$\bar{2}61$	47.64
1.900	8	$\bar{1}33,411$	47.84
1.878	4	$\bar{3}23$	48.42
1.844	2	$\bar{5}11,152$	49.38
1.839	2	421	49.53
1.829	9	440	49.81
1.792	9	123,170	50.93
1.773	2	$\bar{1}62,261$	51.49
1.765	5	$\bar{5}12,\bar{4}13,+$	51.76
1.755	3	351	52.06
1.751	3	431	52.21
1.7161	8	$043,\bar{5}22,+$	53.34
1.6938	5	171,270	54.10
1.6596	1	212	55.31
1.6442	7	$\bar{4}33,\bar{5}32,+$	55.87
1.6319	3	$\bar{4}52,\bar{3}62$	56.33
1.6208	2	$\bar{2}53$	56.75
1.6161	2	342	56.93
1.5981	2	361	57.63
1.5871	5	$271,\bar{1}72$	58.07
1.5779	7	$\bar{5}13,511$	58.44
1.5583	6	370,233	59.25
1.5422	5	$\bar{5}23,460,+$	59.93

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2.6H_2O$, J. Chem. Soc. **63**, 337-423.

Sample

The sample was prepared at NBS by C. W. Reimann. It was precipitated from water solutions of imidazole and $Ni(NO_3)_2$.

Color

Unground - very purplish blue

Optical data

Uniaxial (-) N_e=1.582, N_o=1.594

Structure

Hexagonal, $R\bar{3}$ (148), Z=3, structure determined by Santoro et al.,[1969].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25°C------	12.353 ±.001	14.804 ±.002

Density

(calculated) 1.505 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 3.0

References

Santoro,A., A.D. Mighell, M. Zocchi and C. W. Reimann (1969). The crystal and molecular structure of hexakis(imidazole) nickel(II) nitrate, $(C_3H_4N_2)_6Ni(NO_3)_2$, Acta Cryst. B25, 842-847.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
8.67	20	101	10.19
6.17	50	110	14.34
6.08	100	012	14.56
5.03	3	021	17.60
4.94	3	003	17.94
4.333	6	202	20.48
3.899	35	211	22.79
3.854	40	113	23.06
3.549	30	122	25.07
3.497	25	104	25.45
3.090	3	220	28.87
3.047	2	024	29.29
2.910	6	131	30.69
2.892	8	303	30.89
2.855	9	015	31.30
2.754	5	312	32.48
2.732	4	214	32.75
2.619	8	223	34.21
2.592	6	205	34.57
2.514	1	042	35.68
2.467	1	006	36.39
2.422	3	321	37.08
2.389	6	125	37.61
2.330	8	232	38.60
2.313	5	134	38.90
2.168	2	404	41.63
2.119	4	051	42.64
2.111	5	413	42.80
2.095	2	315	43.15
2.046	2	324	44.23
2.030	2	306	44.59
2.003	3	241	45.24
1.985	2	045	45.67
1.967	1	027	46.11
1.950	3	422	46.54
1.900	3	333	47.83
1.889	2	235	48.13
1.874	1	217	48.54
1.782	2	600	51.22
1.774	2	244	51.46
1.748	1	208,431	52.29
1.734	2	505	52.75
1.722	2	137	53.15
1.713	2	520	53.45
1.696	2	416	54.02

Sample

The sample was prepared by W. S. Brower as a single crystal pulled from a melt. After grinding, the effect of very strong cleavage, {110}, was noted in some sample mountings.

Color

Colorless

Optical data

Biaxial (-) N_α=1.82, N_β=1.83, N_γ=1.84
2V is medium large

Structure

Monoclinic, C2/m (12), Z=8, isostructural with $MnMoO_4$, structure of $MnMoO_4$ determined by Abrahams and Reddy [1965].

Density

(calculated) 3.809 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.6

Polymorphism

Another monoclinic form is described as the high pressure modification, (wolframite type), PDF card 16-308. [Young and Schwartz, 1963].

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.727	4	110,001	13.15
5.323	7	$\bar{1}11$	16.64
4.667	29	$\bar{2}01$	19.00
4.354	3	111	20.38
3.823	46	021	23.25
3.513	25	201	25.33
3.374	100	$\bar{2}20$	26.39
3.283	32	$\bar{1}12$	27.14
3.252	15	$\bar{2}02$	27.40
3.156	20	$\bar{3}11$	28.25
3.091	4	310	28.86
2.795	14	112,$\bar{1}31$	31.99
2.724	6	022	32.85
2.669	13	$\bar{3}12$	33.55
2.663	10	$\bar{2}22$	33.62
2.623	3	131	34.16
2.556	<1	311	35.08
2.460	8	400	36.50
2.322	8	040,$\bar{1}32$	38.74
2.275	2	$\bar{3}31$	39.58
2.252	10	330	40.00
2.176	9	222	41.47
2.128	4	$\bar{1}32$	42.44
2.112	4	$\bar{3}13$	42.79
2.100	3	240	43.04
2.086	8	$\bar{4}22$	43.35
2.080	10	$\bar{2}41$	43.48
2.068	8	$\bar{2}23$	43.73
2.018	5	312,331,+	44.88
2.011	8	113	45.05

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	β(°)
Pakhomov and Medvedev [1968]----	10.35	9.23	7.12	106°30′
NBS, sample at 25 °C----------	10.281 ±.001	9.291 ±.001	7.030 ±.001	106°54′ ±1′

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.966	5	$\bar{4}03$	46.14
1.938	11	241	46.84
1.928	12	421	47.09
1.924	10	510,$\bar{5}$12	47.21
1.911	4	042	47.53
1.890	2	$\bar{2}42$	48.09
1.867	2	$\bar{1}33$	48.74
1.848	2	203	49.27
1.825	2	150	49.94
1.787	2	$\bar{1}51$	51.06
1.755	10	204	52.07
1.739	2	151	52.58
1.720	6	$\bar{4}41$,332	53.21
1.714	8	$\bar{1}14$,$\bar{5}31$	53.42
1.689	10	242,440	54.28
1.678	2	$\bar{6}02$	54.66
1.660	4	530,$\bar{5}$32	55.31
1.646	4	$\bar{4}42$	55.79
1.642	3	$\bar{1}52$,$\bar{2}24$	55.95
1.638	3	$\bar{2}43$	56.09
1.625	2	$\bar{3}51$,$\bar{4}04$	56.59
1.616	4	313,350	56.94
1.612	4	043	57.08
1.607	2	$\bar{6}21$	57.30
1.5811	6	024	58.31
1.5696	2	152	58.78
1.5602	2	114	59.17
1.5457	6	$\bar{3}52$,620	59.78
1.5341	6	$\bar{4}24$	60.28
1.5092	4	061	61.38
1.5006	4	$\bar{4}43$	61.77
1.4960	4	601	61.98
1.4767	6	260	62.88
1.4661	2	204	63.39
1.4505	4	333	64.15
1.4457	6	243,$\bar{7}$11	64.39

References

Abrahams, S.C. and J.M. Reddy(1965). Crystal structure of the transition-metal molybdates. I.paramagnetic alpha-$MnMoO_4$, J. Chem. Phys. 43, No.7, 2533-2543.

Pakhomov, V. I. and A. V. Medvedev (1968). Preliminary data on the crystal structure of magnesium molybdate,Soviet Phys. Cryst. (English Transl.) 12, No.6, 925.

Young, A.P. and C.M. Schwartz (1963).High-pressure synthesis of molybdates with the wolframite structure, Science 141, 348-349.

Sample
Crystals of the hexahydrate were formed very slowly when anhydrous magnesium perchlorate hydrated in a loosely stoppered bottle.

Major impurities
0.001-0.01% each: Ca

Color
Colorless

Optical data
Uniaxial (-) N_o=1.484, N_e=1.468

Structure
Hexagonal, P6/mmm (191), Z=4 or orthorhombic, $Pmn2_1$ (31), Z=2
Structure determined by West, [1935]

Lattice constants

	a(Å)	c(Å)
West [1935]----------	15.55	5.27
NBS, sample at 25 °C-----	15.606 ±.001	5.2788 ±.0005

Density
(calculated) 1.976 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.7

Additional patterns
1. PDF card 14-22 [Hanawalt et al., 1938]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.75	6	200	13.11
4.92	4	101	18.03
4.37	6	111	20.29
4.15	90	201	21.37
3.90	100	220	22.80
3.670	2	211	24.23
3.424	2	301	26.00
3.377	4	400	26.37
3.054	1	311	29.22
2.843	85	401	31.44
2.671	<1	321	33.52
2.638	11	002	33.95
2.573	1	411	34.83
2.552	20	420	35.13
2.458	3	202	36.52
2.332	1	331	38.58
2.297	13	421	39.18
2.292	2	600	40.01
2.205	<1	511	40.90
2.1862	<1	222	41.26
2.0796	4	402	43.48
2.0715	4	601	43.66
2.0474	<1	431	44.20
2.0023	1	521	45.25
1.9501	10	440	46.53
1.9202	1	611	47.30
1.8740	2	620	48.54
1.8354	9	422	49.63
1.8135	<1	531	50.27
1.7872	<1	512	51.06
1.7660	11	621	51.72
1.7134	1	602	53.43
1.7025	2	203,630	53.80
1.6897	1	800	54.24
1.6440	<1	541	55.88
1.6208	<1	631	56.75
1.6089	1	801	57.21
1.5931	<1	313	57.83
1.5684	<1	442	58.83
1.5609	3	403,550	59.14
1.5499	<1	640	59.60

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.5283	2	622	60.53
1.4874	4	641	62.38
1.4746	4	503,820	62.98
1.4493	<1	423	64.21
1.4451	<1	901	64.42
1.4229	2	802	65.55
1.4200	2	821	65.70
1.3866	1	603	67.49
1.3686	<1	651	68.50
1.3550	1	741	69.29
1.3517	1	10·0·0	69.48
1.3378	<1	613	70.31
1.3005	4	533,660	72.64
1.2829	1	623,10·1·0	73.80
1.2503	1	224	76.06
1.2412	1	841	76.72
1.2184	<1	803	78.43
1.2161	<1	931	78.60
1.2032	<1	10·0·2	79.61
1.1829	2	10·2·1	81.26
1.1665	1	662	82.65
1.1634	1	643	82.92
1.1496	<1	842	84.14
1.1388	<1	604	85.13
1.1263	<1	524,12·0·0	86.30
1.1027	<1	10·2·2	88.62
1.0931	<1	444	89.61
1.0872	<1	861	90.22
1.0820	1	833,10·4·0	90.78

References

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-513.

West, C.D. (1935). Crystal structures of hydrated compounds. II structure type $Mg(ClO_4)_2 \cdot 6H_2O$, Z.Krist. (A)91,480-493

Sample

The sample was obtained from Mallinckrodt Chemical Works.

Major impurities

trace amounts of Fe, Ca, Cr, and Mg.

Color

Orange-red

Structure

Tetragonal, $P4_2/nmc$ (137), Z=2, structure determined by Bijvoet et al.,[1926].

Lattice constants

	a(Å)	c(Å)
Havighurst* [1925]--------	4.356	12.34
Bijvoet et al.* [1926]----	4.357	12.36
Huggins and Magill*[1927]-	4.34	12.34
Swanson and Tatge [1953]--	4.390	12.38
Vlasse [1963]-------------	4.361	12.450
NBS, sample at 25 °C------	4.3693	12.4399
	±.0001	±.0004

*values as published

Density

(calculated) 6.354 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

Polymorphism

Goya et al.[1962] reported a yellow, orthorhombic form stable above 127 °C. Vlasse [1963] also notes a metastable orange, cubic or pseudo cubic form.

Additional patterns

1. Havighurst [1925]
2. Hanawalt, Rinn, and Frevel [1938]
3. PDF card 4-454 [Swanson and Tatge,1953]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.223	55	002	14.22
4.122	70	101	21.54
3.577	100	102	24.87
3.113	3	004	28.65
3.092	2	110	28.85
3.009	40	103	29.66
2.768	30	112	32.32
2.534	7	104	35.39
2.192	60	114	41.14
2.186	55	200	41.27
2.163	17	105	41.73
2.074	14	006	43.60
2.062	6	202	43.87
1.931	9	211	47.02
1.874	15	106	48.55
1.865	14	212	48.79
1.789	1	204	51.02
1.768	6	213	51.65
1.722	1	116	53.14
1.6543	3	214	55.50
1.6464	5	107	55.79
1.5554	5	008	59.37
1.5450	4	220	59.81
1.5371	5	215	60.15
1.5039	6	206	61.62
1.4655	2	108	63.42
1.4469	2	301	64.33
1.4221	4	216	65.59
1.4181	5	302	65.80
1.3745	2	303	68.17
1.3490	2	312	69.64
1.3176	3	109	71.55
1.3144	4	217	71.75
1.2669	5	208	74.89
1.2629	7	314	75.17
1.2570	3	305	75.58
1.2389	2	226	76.89
1.2168	1	218	78.55
1.2061	1	321	79.38
1.1966	1	1·0·10	80.14

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.1917	2	3·0·6	80.54
1.1895	2	322	80.72
1.1631	1	323	82.95
1.1542	3	1·1·10	83.73
1.1285	1	219	86.09
1.0958	2	228	89.33
1.0926	2	400	89.66
1.0893	1	325	90.00
1.0759	1	402	91.44
1.0630	1	308	92.88
1.0559	1	411	93.69
1.0494	1	2·1·10	94.45
1.0462	1	326	94.83
1.0448	2	412	95.00
1.0266	1	413	97.24
1.0160	<1	332	98.60
1.0087	1	1·0·12	99.57
1.0027	<1	309	100.38
0.9828	2	1·1·12	103.21
.9777	1	334	103.97
.9770	2	319,420	104.08
.9664	1	406	105.70
.9435	1	416	109.45
.9244	2	3·1·10	112.87
.9157	2	2·1·12	114.54
.9101	2	417	115.63
.8938	2	408	119.03
.8838	1	426	121.27
.8653	<1	432	125.79
.8550	1	433,511	128.56
.8489	2	512	130.29
.8291	1	3·1·12	136.56
.8272	2	428	137.25
.8261	1	514	137.63
.8067	<1	4·1·10	145.44
.8052	<1	436	146.12
.8045	<1	522	146.43
.7963	<1	523	150.63
.7933	1	3·3·10	152.32
.7878	2	3·2·12	155.82

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Vlasse, Marcus (1963) The structure of the crystalline phases in the mercuric iodide system, 21st Annual Pittsburgh Diffraction Conference, (Abstracts).

Sample

The sample was prepared at NBS by melting a stoichiometric mixture of K_2SO_4 and $CdSO_4$ and annealing for 18 hours at 300 °C and then for 3 days at 150 °C.

Major impurities

0.001-0.01% each: Na

0.01 -0.1 % each: Ca and Al

Color

Yellowish white

Optical data

Very low double refraction. N_α=1.588 and N_γ=1.592 (data limited by small grain size of the sample).

Structure

Orthorhombic, probably $P2_12_12_1$ (19), Z=4 Distorted langbeinite-type. A cubic cell was reported by Gattow and Zemann [1958]

Lattice constants

	a(Å)	b(Å)	c(Å)
Gattow and Zemann [1958]--	10.28 ±.05		
NBS, sample at 25 °C----------	10.212 ±.001	10.280 ±.001	10.171 ±.001

Density

(calculated) 3.677 g/cm³ at 25 °C.

Reference intensity

$I/I_{corundum}$ = 2.7

Polymorphism

DTA measurements show a reversible inversion at 166 °C. This is interpreted as a change to the undistorted langbeinite structure on heating.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.23	<1	110,011	12.23
5.90	33	111	15.00
5.11	3	200	17.34
4.572	35	210,201	19.40
4.184	22	121	21.22
3.607	4	202	24.66
3.413	27	221,122	26.09
3.245	80	130,031	27.46
3.227	100	310,301	27.62
3.216		013,103	27.72
3.094	15	131	28.83
3.077	22	311	28.99
2.841	8	032,320	31.46
2.830	12	023,302	31.59
2.737	82	231,132,+	32.69
2.727		312,123,+	32.81
2.568	4	040	34.91
2.551	<1	400	35.15
2.483	8	232	36.15
2.475	12	401,223	36.27
2.468	8	014,104	36.37
2.404	3	303	37.38
2.346	10	133	38.33
2.340	8	313	38.44
2.295	3	240,042	39.22
2.276	<1	024,204	39.57
2.237	11	241,142	40.28
2.231	8	421	40.40
2.226		412,124	40.49
2.176	12	323	41.46
2.092	15	242	43.21
2.084	28	422	43.38
2.081		224	43.46
2.051	5	340	44.12
2.039	11	403	44.39
2.016	10	150,051	44.92
2.009	28	143,431	45.10
2.001	32	413	45.29
1.977	6	151	45.85
1.966	8	333,511	46.13
1.959		115	46.31
1.906	5	250,052	47.68
1.896	22	234,423,+	47.93
1.890		025,205	48.09
1.875	1	251,152	48.52
1.865	2	521,512	48.79

Internal standard W, a = 3.16516 Å CuKα_1, λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.802	1	404	50.62
1.783	8	441	51.20
1.778		522	51.33
1.775	8	414,225	51.45
1.760	4	350	51.91
1.755	5	343,530	52.07
1.749	5	503,035	52.26
1.734	3	351,153	52.75
1.729	2	531	52.90
1.725	1	513,135	53.05
1.706	1	442	53.67
1.690	2	160,061	54.24
1.678	3	610,601	54.65
1.666	9	161	55.06
1.663	17	352,253	55.20
1.658	12	532,611	55.38
1.650	13	116	55.64
1.624	6	260,062	56.61
1.614	<1	602	57.01
1.609	6	026,206	57.20
1.605	6	261,162	57.37
1.597	6	443,344,+	57.69
1.591	<1	405,126,+	57.93
1.579	8	541,154	58.38
1.575	8	145	58.55
1.573	7	514,415	58.63
1.558	3	533	59.26
1.539	3	622	60.05
1.535	2	226	60.23
1.527	3	452	60.57
1.524	3	630	60.71
1.520	<1	425,036	60.91
1.514	2	361	61.16
1.508	2	631	61.45
1.504	5	136	61.63
1.475	5	444	62.95
1.465	4	362,263	63.42
1.459	<1	632,623	63.72
1.455	4	326	63.92
1.444	5	701,534,+	64.48

References

Gattow,G.and J.Zemann (1958). Über Doppelsulphate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$ Z. Anorg. Allgem. Chem. **293**, 233-240.

Sample

The sample was prepared by melting a mixture of KCl and anhydrous $CaCl_2$ at 750 °C. The material is hygroscopic and the patterns were made with the sample enclosed in a dry-mount.

Color

Colorless

Optical data

Very low birefringence, N=1.568, shows polysynthetic twinning.

Structure

Orthorhombic, Pnma (62), Z=4, by analogy with $NaZnF_3$ and similar distorted perovskites.

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C---------	7.551 ±.001	10.442 ±.001	7.251 ±.001

Density

(calculated) 2.155 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 1.0$

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.227	25	101,020	16.95
4.679	6	111	18.95
3.776	9	200	23.54
3.697	30	121	24.05
3.622	5	002	24.56
3.348	7	201	26.60
3.270	12	102	27.25
3.188	14	211	27.96
3.137	35	031	28.43
3.119	30	112	28.60
3.058	18	220	29.18
2.978	12	022	29.98
2.896	14	131	30.85
2.819	13	221	31.72
2.770	8	122	32.29
2.614	100	202	34.27
2.610		040	34.33
2.559	7	230	35.03
2.537	10	212	35.35
2.414	4	231	37.21
2.377	15	301	37.82
2.338	13	222,141	38.48
2.318	13	311	38.81
2.248	4	113	40.07
2.163	8	321	41.72
2.146	13	240	42.06
2.119	14	042	42.64
2.107	25	123	42.89
2.037	5	203	44.45
2.006	3	051	45.16
1.963	3	331	46.21
1.920	4	133	47.31
1.887	5	400	48.19
1.857	2	410	49.00
1.847	12	242	49.30
1.827	6	250,401	49.87
1.812	1	004	50.31
1.778	7	332	51.35
1.772	10	251	51.52
1.758	10	341,233	51.97
1.744	1	303	52.43
1.740	<1	060	52.55
1.720	<1	313	53.21
1.674	<1	402	54.81
1.670	2	124	54.94
1.652	3	161	55.59
1.632	4	252	56.32
1.615	<1	214	56.96
1.606	<1	243	57.34
1.569	1	351,062	58.80
1.559	2	224,333	59.22
1.547	2	153	59.74
1.530	2	440	60.45
1.509	3	432	61.40
1.489	1	044	62.30
1.479	2	234,501	62.78
1.474	<1	413	63.03
1.464	1	511	63.49
1.461	1	071,144	63.64
1.434	<1	171	64.96
1.4311	1	423	65.13
1.4164	<1	324	65.89
1.4103	<1	115	66.21
1.3998	<1	450	66.77

Sample

The $K_2CaMg(SO_4)_3$ was prepared by melting a stoichiometric mixture of K_2SO_4, $CaSO_4$, and $MgSO_4$. The sample was annealed for 20 hours at 800°C and 17 hours at 400°C.

Major impurities

0.01 -0.1 % each: Cs, Cu, Na, and Rb

0.1 -1.0 % each: Fe

Color

Yellowish white

Optical data

Isotropic, N=1.525

Structure

Cubic, $P2_13$ (198), Z=4 by analogy with langbeinite, $K_2Mg_2(SO_4)_3$. The langbeinite structure was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
NBS, sample at 25°C----------	10.1662 ±.0003

Density

(calculated) 2.723 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.6

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.86	4	111	15.11
4.544	1	210	19.52
4.149	21	211	21.40
3.596	<1	220	24.74
3.388	2	221	26.28
3.212	100	310	27.75
3.066	9	311	29.10
2.819	7	320	31.72
2.717	34	321	32.94
2.540	<1	400	35.30
2.466	4	322	36.40
2.333	2	331	38.56
2.273	1	420	39.61
2.219	2	421	40.63
2.168	4	332	41.63
2.075	7	422	43.59
2.033	1	430	44.54
1.994	10	510	45.45
1.957	1	511	46.35
1.888	4	520	48.16
1.856	1	521	49.04
1.769	3	522	51.61
1.743	1	530	52.44
1.718	<1	531	53.27
1.695	<1	600	54.06
1.671	1	610	54.90
1.649	8	611	55.69
1.608	2	620	57.26
1.588	2	621	58.04
1.569	2	541	58.82

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.550	<1	533	59.58
1.532	<1	622	60.37
1.5154	2	630	61.10
1.4986	2	631	61.86
1.4678	1	444	63.31
1.4522	1	632	64.07
1.4380	<1	550	64.78
1.4096	1	640	66.25
1.3967	1	720	66.94
1.3834	2	721	67.67
1.3586	1	642	69.08
1.3468	<1	722	69.77
1.3348	<1	730	70.49
1.3234	1	731	71.19
1.3014	1	650	72.58
1.2909	1	732	73.27
1.2612	1	810	75.29
1.2517	<1	811	75.96
1.2423	<1	733	76.64
1.2328	<1	820	77.34
1.2240	<1	821	78.00
1.2154	<1	653	78.66
1.1985	<1	822	79.99
1.1817	1	831	81.36
1.1740	<1	751	82.01
1.1513	<1	752	83.99
1.1290	<1	841	86.04
1.1223	<1	910	86.68
1.1158	<1	911	87.31
1.1090	<1	842	87.99
1.0961	1	921	89.30
1.0836	<1	664	90.61
1.0774	<1	922	91.28
1.0717	<1	930	91.90
1.0545	<1	852	93.85

References

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Sample

The sample was prepared at NBS by melting a stoichiometric mixture of K_2SO_4 and $CaSO_4$. This was then annealed for 18 hours at 700 °C.

Major impurities

0.01 -0.1 % each: Ag and Cu.

0.1 -1.0 % each: Cs and Na.

Color

Colorless.

Optical data

Biaxial(-) N_α=1.522, N_β=1.526, N_γ=1.527, 2V is small.

Structure

Orthorhombic, probably $P2_12_12_1$ (19), Z=4. Distorted langbeinite type. $K_2Ca_2(SO_4)_3$ has been reported as cubic [Ramsdell, 1935].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
Ramsdell [1935]--	10.35		
NBS, sample at 25° C----------	10.334 ±.001	10.501 ±.001	10.186 ±.001

Density

(calculated) 2.683 g/cm³ at 25 °C.

Reference intensity

$I/I_{corundum}$ = 0.9

Polymorphism

Inverts to a cubic langbeinite form at 200 °C [Morey et al.,1964]. An inversion at 940 °C has also been reported [Bellanca,1942].

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
7.32	4	011	12.08
5.969	8	111	14.83
4.665	3	021	19.01
4.574	6	012,102	19.39
4.255	28	121	20.86
4.221	23	211	21.03
4.189	16	112	21.19
3.462	12	221	25.71
3.315	93	130,031	26.87
3.272	79	310	27.23
3.263		301	27.31
3.225	100	013,103	27.64
3.152	18	131	28.29
3.116	18	311	28.62
3.082	3	113	28.95
2.987	2	222	29.89
2.881	18	032,320	31.02
2.853	6	302,023	31.33
2.786	43	231	32.10
2.776	49	132	32.22
2.750	43	312,123	32.53
2.743		213	32.62
2.543	6	140,041	35.26
2.510	4	410,322	35.75
2.497	4	223	35.93
2.471	4	104,141	36.32
2.436	2	033,411	36.86
2.406	2	114	37.35
2.387	3	331	37.65
2.372	7	133	37.90
2.357	2	313	38.15
2.341	2	240	38.42
2.333	2	042	38.55
2.276	5	142	39.56
2.250	2	412	40.04
2.232	3	214	40.38
2.213	4	332	40.74
2.204	8	233	40.91
2.196	11	323	41.07
2.125	4	242	42.50
2.109	18	422	42.84

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.093	22	224	43.18
2.058	8	150,051,+	43.97
2.044	6	341	44.27
2.037	14	431,143	44.44
2.018	19	413,151,+	44.88
2.010	14	314	45.06
1.990	4	333,511	45.55
1.941	2	052	46.75
1.932	5	342	47.00
1.924	6	432,520	47.21
1.914	6	502,423,+	47.46
1.908	4	152,324	47.62
1.891	3	521	48.08
1.884	1	512	48.26
1.818	2	252	50.14
1.811	6	441	50.33
1.799	2	144,522	50.71
1.793	3	350	50.88
1.786	4	414,053	51.09
1.780	4	530,343	51.27
1.765	2	503,035	51.75
1.753	2	305,531	52.13
1.730	2	315	52.89
1.725	2	160,061	53.04
1.700	6	161,610	53.87
1.697	6	601,006	53.98
1.692	8	352	54.17
1.688	8	253	54.30
1.675	5	016,106,+	54.74
1.664	4	325	55.16
1.654	5	062,116	55.51
1.635	2	162	56.22
1.631	2	602	56.35
1.610	7	434,045	57.15
1.604	6	504,541	57.40
1.600	4	154,405	57.55
1.594	2	216	57.78

Additional patterns

1.PDF card 17-0741 [Morey et al.,1964]

References

Bellanca,A.(1942) L'aftitalite nel sistema ternario K_2SO_4-Na_2SO_4-$CaSO_4$, Periodico Mineral.(Rome) **13**, 21-85.

Morey, G.W., J.J. Rowe, and R.O. Fournier (1964). The system $K_2Mg_2(SO_4)_3$ (langbeinite) - $K_2Ca_2(SO_4)_3$ (calcium-langbeinite), J. Inorg. Nucl. Chem. **26**, 53-58.

Ramsdell, L.S. (1935). An x-ray study of the system K_2SO_4-$MgSO_4$-$CaSO_4$, Am. Mineralogist. **20**, 569-574.

Sample

The sample was crystallized from a mixture of concentrated hydrochloric acid, KCl and $CuCl_2$ by dehydration in a desiccator.

Major impurities

less than 0.001% each of Al, Ba, Ca, Mg, and Si

Color

Strong brown

Optical data

Anisotropic, N_α=1.670, N_γ=1.890. Crystals were very fine and needle shaped.

Structure

Monoclinic, $P2_1/c$ (14), Z=4, Structure determined by Willett et al. [1963]

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
Willett et al.-[1963]	4.029 ±.005	13.785 ±.003	8.736 ±.004	97°20′ ± 5′
NBS sample at 25 °C	4.031 ±.001	13.788 ±.002	8.732 ±.001	97°10′ ± 1′

Density

(calculated) 2.883 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.0

References

Willett, R. D., C. Dwiggins,Jr.,R. F. Kruh and R. E. Rundle (1963). Crystal structures of $KCuCl_3$ and NH_4CuCl_3. J. Chem. Phys. 38, 2429-2436.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.33	65	011	12.06
6.89	100	020	12.84
5.40	55	021	16.41
4.33	14	002	20.47
4.13	30	012	21.48
4.06	40	031	21.87
3.67	75	022	24.20
3.45	8	040	25.81
3.366	15	111	26.46
3.342	12	$\bar{1}21$	26.65
3.178	80	$\bar{1}02$	28.42
3.061	95	$\bar{1}12$	29.15
2.937	15	$\bar{1}31$	30.41
2.856	90	$\bar{1}22$	31.29
2.772	40	102,131	32.27
2.714	90	112	32.98
2.698	75	042	33.18
2.665	40	023	33.60
2.629	60	051	34.07
2.572	60	122	34.85
2.454	6	$\bar{1}13$	36.58
2.374	25	132	37.87
2.346	30	$\bar{1}23$	38.34
2.326	17	052	38.67
2.271	45	150	39.66
2.222	45	061	40.57
2.215	45	043	40.69
2.186	11	113	41.26
2.158	13	142,151	41.83
2.142	4	014	42.16
2.110	12	123	42.83
2.066	20	024	43.77
2.020	17	$\bar{1}43$	44.83
2.001	40	200	45.29
1.959	25	034	46.30
1.932	12	$\bar{1}24$	46.99
1.921	20	071	47.28
1.863	30	143	48.84
1.850	17	$\bar{1}53$	49.22
1.844	16	$\bar{1}34$	49.38
1.792	18	072	50.90
1.767	17	170	51.69
1.750	19	$\bar{1}71$	52.21
1.703	9	054	53.78

Sample

The sample was prepared by adding hydrofluoric acid to a mixture of K_2CO_3 and $NiCO_3$. The material was then heated to about 200 °C.

Color

Pale yellow green

Structure

Cubic, perovskite type, Pm3m (221) Z=1 [Rüdorff et al., 1958]. $KNiF_3$ was reported by Martin et al., [1956] as pseudocubic.

Lattice constants

	a(Å)
Martin et al.[1956]----------	4.01*
Rüdorff et al.[1959]----------	4.009
Hirakawa et al.[1960]----------	4.015 ±.001
Okazaki and Suemune[1961]-------	4.014 ±.001
Knox [1961]----------	4.012
NBS, sample at 25 °C----------	4.0127 ±.0001

*pseudocubic

Density

(calculated) 3.978 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.0$

Additional patterns

1.PDF card 1-0985 Dow Chemical Co., Midland, Michigan.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.02	30	100	22.12
2.84	100	110	31.48
2.317	12	111	38.83
2.006	65	200	45.15
1.795	11	210	50.83
1.639	30	211	56.07
1.418	25	220	65.80
1.3376	4	300	70.32
1.2686	10	310	74.77
1.2096	2	311	79.11
1.1581	8	222	83.38
1.1129	2	320	87.60
1.0726	9	321	91.80
1.0032	4	400	100.32
.9732	2	410	104.65
.9457	6	411	109.08
.9206	2	331	113.59
.8973	8	420	118.29
.8757	2	421	123.20
.8554	4	332	128.45
.8190	5	422	140.27
.7870	3	510	156.35

References

Hirakawa, K., K.Hirakawa and T. Hashimoto (1960). Magnetic properties of potassium iron group fluorides, KMF_3, J.Phy. Soc. Japan 15, 2063-2068.

Knox, K.(1961). Perovskite-like fluorides, I. Structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$, and $KZnF_3$. Crystal field effects in the series and in $KCrF_3$ and $KCuF_3$, Acta Cryst. 14, 583-585.

Martin, R.L., R.S. Nyholm and N. C. Stephenson (1956). Antiferromagnetism in complex fluorides with perovskite structure Chem. Ind. (London) 1956, 83-85.

Okazaki,A. and Y. Suemune(1961). The crystal structures of $KMnF_3$, $KFeF_3$, $KCoF_3$, $KNiF_3$ and $KCuF_3$ above and below their Néel temperatures, J. Phys. Soc. Japan 16, 671-675.

Rüdorff, W., J. Kändler, G. Lincke and D. Babel (1959). Über Doppelfluoride von Nickel und Kobalt, Angew. Chem. 71, 672.

Sample

The sample was prepared at NBS by slow evaporation of an equimolar solution of K_2SO_4 and $ZnSO_4$.

Major impurities

less than 0.001 % each: Ca, Cu, Li, Mg, Mn, Rb, and Si

Color

Colorless

Optical data

Biaxial(+) N_α=1.478, N_β=1.481, N_γ=1.496
2V is large

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other"Tutton's salts"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
Kohler, Franke* [1965]	9.04	12.20	6.15	104°48′
NBS, sample at 25 °C	9.041 ±.001	12.215 ±.001	6.156 ±.001	104°49′ ±1′

*PDF card 18-1074

Density

(calculated) 2.242 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.3

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.12	14	020	14.46
5.96	6	001	14.86
5.35	12	011	16.57
5.13	12	$\bar{1}11$	17.28
5.00	4	120	17.72
4.38	25	200	20.27
4.265	28	021	20.81
4.154	87	111	21.37
4.051	82	$\bar{2}01$	21.92
3.845	4	$\bar{2}11$	23.11
3.691	100	130	24.09
3.581	10	121	24.84
3.552	10	220	25.05
3.374	4	$\bar{2}21$	26.39
3.362	12	031	26.49
3.303	25	$\bar{1}31$	26.97
3.159	18	201	28.23
3.058	41	211,040	29.18
2.975	64	002,$\bar{1}12$	30.01
2.872	4	$\bar{2}31$	31.11
2.846	8	$\bar{3}11$	31.40
2.832	17	310	31.56
2.806	29	221	31.86
2.742	21	$\bar{1}22$	32.63
2.684	7	$\bar{1}41$	33.35
2.640	7	$\bar{3}21$	33.93
2.557	6	$\bar{2}22$	35.06
2.513	5	141	35.70
2.502	10	240	35.86
2.495	13	231	35.97
2.448	<2	$\bar{1}32$	36.68
2.406	5	122	37.34
2.401		032	37.43
2.380	46	$\bar{3}31$	37.77
2.260	7	051	39.86
2.244	6	$\bar{4}01$,322,+	40.15
2.203	9	132	40.93
2.195	23	241	41.09
2.176	<2	212	41.46
2.150	3	410	41.98

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.137	16	151	42.26
2.131		250,042	42.37
2.114	<2	$\bar{3}41$	42.73
2.107	4	340,$\bar{4}21$	42.88
2.093	3	$\bar{2}51$	43.19
2.071	12	$\bar{2}42$	43.66
2.058	14	331,420	43.95
2.037	<2	060	44.44
2.024		$\bar{4}02,\bar{1}13$	44.74
2.010	2	$\bar{2}03$	45.07
1.984	13	003,$\bar{2}13$	45.69
1.945	<2	$\bar{1}23$,232	46.67
1.932	2	251	47.00
1.926	5	061,430	47.16
1.910	<2	$\bar{1}52,\bar{2}23$	47.57
1.893	6	$\bar{3}42$	48.03
1.889	8	052	48.14
1.876	8	411,$\bar{3}51$	48.49
1.871	8	350	48.61
1.856	8	$\bar{3}13$	49.03
1.849	3	161	49.23
1.831	6	$\bar{1}33$	49.75
1.820	8	$\bar{2}61$	50.09
1.815	4	113,421,+	50.23
1.803	5	$\bar{2}33$	50.59
1.783	7	033	51.18
1.776	8	322,440	51.41
1.758	2	123	51.96
1.731	6	510	52.85
1.722	<2	431	53.15
1.707	3	351,$\bar{3}33$	53.66
1.696	2	$\bar{1}62$	54.02
1.691	4	332	54.21
1.680	4	520,062,+	54.58
1.674	4	071,133	54.79
1.654	<2	203,$\bar{4}51$	55.51
1.650	<2	$\bar{2}62$	55.66
1.639	<2	213,$\bar{4}23$,+	56.07
1.628	2	450	56.46
1.623	4	171	56.68

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.608	2	162	57.23
1.597	<2	223	57.68
1.577	3	$\bar{5}32$	58.47
1.566	<2	412	58.93
1.559	<2	$\bar{4}52$,511	59.20
1.555	<2	$\bar{5}41$	59.39
1.539	<2	053	60.05
1.533	2	$\bar{2}04$,233	60.32
1.522	<2	$\bar{2}14,\bar{1}14$	60.83
1.517	2	540,$\bar{1}72$	61.05
1.505	2	072,$\bar{1}80$	61.59
1.496	<2	370,$\bar{6}11$	62.00
1.486	2	$\bar{1}24,\bar{4}43$	62.46
1.474	<2	$\bar{1}81,\bar{5}23$	63.02
1.472	<2	432	63.09
1.467	<2	153,531	63.35
1.463	<2	313,$\bar{6}21$	63.52
1.452	<2	$\bar{5}51,\bar{1}72$	64.06
1.445	<2	024,$\bar{1}63$,+	64.42

Additional patterns

1. PDF card 1-421, [Hanawalt et al., 1938]
2. PDF card 18-1074, [Kohler and Franke, 1965]

References

Hanawalt, J.D., H.D. Rinn, and L.K. Frevel (1938). Chemical analyses by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-512.

Kohler, K. and W. Franke (1965). Mineralogisches Institut Freie Universität, Berlin, Germany.

Margulis, T. N. and D.H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 344-357.

Tutton, A. E.(1893).Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series.A study of the potassium, rubidium, and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)\cdot 6H_2O$, J. Chem. Soc. 63, 337-423.

Sample

The sample was prepared by melting a stoichiometric mixture of Rb_2SO_4 and $3CdSO_4 \cdot 8H_2O$, which was then air quenched and annealed at 700 °C for 18 hours.

Color

Colorless

Optical data

Isotropic, N=1.590

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann,1958]. The langbeinite structure was determined by Zemann and Zemann, [1957].

Lattice constants

	a(Å)
Gattow and Zemann[1958]---------	10.382
NBS, sample at 25 °C----------	10.3810 ±.0002

Density

(calculated) 4.060 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 5.3

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.98	4	111	14.80
4.64	9	210	19.12
4.23	15	211	20.96
3.669	5	220	24.24
3.460	2	221	25.73
3.283	100	310	27.14
3.130	11	311	28.50
2.881	5	320	31.02
2.773	65	321	32.25
2.593	1	400	34.56
2.517	3	410	35.64
2.380	2	331	37.76
2.321	1	420	38.77
2.265	1	421	39.77
2.214	4	332	40.72
2.119	24	422	42.63
2.076	3	430	43.57
2.037	31	510	44.44
1.997	4	511	45.38
1.927	7	520	47.11
1.895	1	521	47.97
1.806	5	522	50.48
1.779	3	530	51.30
1.706	2	610	53.68
1.6840	19	611	54.44
1.6413	8	620	55.98
1.6208	6	621	56.75
1.6017	8	541	57.49
1.5476	3	630	59.70
1.5304	6	631	60.44
1.4978	3	444	61.90
1.4829	3	632	62.59
1.4680	3	710	63.30
1.4538	1	711	63.99
1.4397	1	640	64.69
1.4260	2	720	65.39
1.4126	5	721	66.09
1.3874	2	642	67.45
1.3748	1	722	68.15
1.3631	2	730	68.82

Internal standard Ag, a = 4.08641 Å $CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.3514	2	731	69.50
1.3291	1	650	70.84
1.3182	3	732	71.51
1.2971	1	800	72.86
1.2877	2	810	73.48
1.2779	1	811	74.14
1.2684	2	733	74.79
1.2598	<1	820	75.43
1.2499	1	821	76.09
1.2409	1	653	76.74
1.2236	4	822	78.03
1.2148	1	830	78.70
1.2068	5	831	79.33
1.1990	2	751	79.95
1.1827	1	832	81.28
1.1754	3	752	81.89
1.1534	1	841	83.80
1.1465	<1	910	84.42
1.1395	1	911	85.06
1.1261	1	920	86.32
1.1196	2	921	86.94
1.1068	1	664	88.21
1.1003	2	922	88.86
1.0943	3	930	89.48
1.0882	1	931	90.12
1.0767	1	852	91.35
1.0706	1	932	92.02
1.0596	1	844	93.26
1.0541	<1	940	93.90
1.0486	1	941	94.54
1.0434	1	933	95.16
1.0331	2	10·1·0	96.42
1.0278	1	10·1·1	97.09
1.0179	1	10·2·0	98.35
1.0130	1	10·2·1	99.00
1.0083	1	950	99.62

References

Gattow,G.and J.Zemann (1958). Über Doppelsulfate vom Langbeinit-typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Sample

The material was made by melting a stoichiometric mixture of RbCl and $CaCl_2$. The sample was very hygroscopic.

Color

Colorless

Optical data

Very low birefringence, N≅ 1.576, polysynthetic twinning was noted.

Structure

Orthorhombic, distorted perovskite, Pnma (62), Z=4, by analogy with $NaZnF_3$.

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C	7.541 ±.001	10.667 ±.001	7.469 ±.001

Density

(calculated) 2.564 g/cm³ at 25° C.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.751	5	111	18.66
3.765	85	200,121	23.61
3.740	25	002	23.77
3.557	3	210	25.01
3.366	6	201	26.46
3.351	7	102	26.58
3.208	12	031,211	27.79
3.194	11	112	27.91
3.077	45	220	28.99
3.059	45	022	29.17
2.952	7	131	30.25
2.846	9	221	31.41
2.837	13	122	31.51
2.667	65	040	33.58
2.653	100	202	33.75

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.588	5	230	34.63
2.577	7	212	34.79
2.443	5	231	36.76
2.438	4	132	36.84
2.382	3	141,301	37.73
2.326	9	311	38.68
2.307	3	113	39.01
2.174	30	321	41.50
2.163	45	123	41.73
2.086	3	142,302	43.34
2.078	3	203	43.52
2.052	3	051	44.10
2.039	2	033,213	44.39
1.978	4	151,331	45.83
1.882	35	242	48.33
1.866	8	004	48.75
1.827	1	401	49.86
1.812	2	104	50.32
1.800	4	152,332	50.68
1.745	1	313	52.40
1.730	2	421	52.88
1.686	8	161	54.38
1.683	7	402	54.47
1.663	2	252,412	55.20
1.615	2	134	56.98
1.605	4	062,422	57.38
1.585	4	153,333	58.16
1.539	3	440	60.05
1.529	3	044	60.50
1.521	4	432	60.86
1.465	2	511,171	63.45
1.447	2	423	64.31
1.4429	2	324	64.53
1.4235	4	442	65.52
1.4208	4	163	65.66
1.4133	6	270,125,+	66.05
1.3865	<1	172,512	67.50
1.3646	2	531	68.73
1.3333	2	080	70.58
1.2569	5	280,600	75.59
1.2539	5	363,523	75.80
1.2482	4	325,610	76.21
1.1917	3	282,602	80.54
1.1878	3	444	80.86
1.1310	2	290,165	85.85

Sample

The material was prepared by melting a 1:2 mixture of Rb_2SO_4 and $CaSO_4$. This was followed by quenching in air, grinding, and then annealing at 650 °C for several days.

Color

Colorless

Optical data

Isotropic, N=1.520

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The langbeinite structure was described by Zemann and Zemann, [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]--------	10.57
NBS, sample at 25 °C----------	10.5687 ±.0002

Density

(calculated) 3.034 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.6$

References

Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z.Anorg. Allgem. Chem. 293, 233-240.

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.09	4	111	14.54
4.726	2	210	18.76
4.312	6	211	20.58
3.734	5	220	23.81
3.519	3	221	25.29
3.340	100	310	26.67
3.185	11	311	27.99
2.928	12	320	30.50
2.821	45	321	31.69
2.641	2	400	33.91
2.564	12	410	34.97
2.424	4	331	37.05
2.364	1	420	38.03
2.306	3	421	39.03
2.252	7	332	40.00
2.157	12	422	41.85
2.113	2	430	42.75
2.073	20	510	43.63
2.033	1	511	44.52
1.963	5	520	46.22
1.929	1	521	47.06
1.840	3	522	49.51
1.813	1	530	50.28
1.787	1	531	51.06
1.760	1	600	51.90
1.738	2	610	52.63
1.714	12	611	53.42
1.6710	5	620	54.90
1.6502	5	621	55.65
1.6311	4	541	56.36
1.6120	1	533	57.09
1.5931	1	622	57.83
1.5752	4	630	58.55
1.5580	4	631	59.26
1.5251	2	444	60.67
1.5096	2	632	61.36
1.4943	1	710	62.06
1.4799	1	711	62.73
1.4651	1	640	63.44
1.4516	1	720	64.10
1.4380	4	721	64.78

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.4122	2	642	66.11
1.3997	1	722	66.78
1.3879	1	730	67.42
1.3755	2	731	68.11
1.3531	1	650	69.40
1.3421	2	732	70.05
1.3211	<1	800	71.35
1.3106	1	810	71.99
1.3010	1	811	72.61
1.2912	1	733	73.25
1.2820	1	820	73.86
1.2724	2	821	74.51
1.2633	1	653	75.14
1.2454	1	822	76.41
1.2370	1	830	77.03
1.2288	2	831	77.64
1.2203	1	751	78.28
1.2047	1	832	79.49
1.1966	1	752	80.14
1.1741	1	663	82.00
1.1601	1	911	83.21
1.1533	1	842	83.81
1.1465	1	920	84.42
1.1397	1	921	85.04
1.1270	1	664	86.23
1.1202	2	922	86.89
1.1140	2	930	87.49
1.1080	1	931	88.09
1.0958	1	852	89.33
1.0900	1	932	89.93
1.0732	1	940	91.74
1.0674	1	941	92.38
1.0624	1	933	92.94
1.0568	1	10·0·0	93.58
1.0516	1	10·0·1	94.19
1.0466	1	10·1·1	94.78
1.0364	1	10·2·0	96.01
1.0316	1	10·2·1	96.61
1.0267	1	950	97.22

Sample

The sample was prepared by melting a stoichiometric mixture of Rb_2SO_4 and $MgSO_4 \cdot 7H_2O$. The melt was cooled quickly and annealed at 800 °C for 18 hours.

Color

Colorless

Optical data

Isotropic, N=1.556

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite type [Gattow and Zemann, 1958]. The langbeinite structure was determined by Zemann and Zemann, [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]--------	10.005
NBS, sample at 25 °C----------	10.0051 ±.0003

Density

(calculated) 3.367 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.3$

References

Gattow, G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Zemann, A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.76	6	111	15.36
4.47	7	210	19.86
4.086	6	211	21.73
3.537	5	220	25.16
3.336	6	221	26.70
3.162	100	310	28.20
3.015	22	311	29.60
2.890	3	222	30.92
2.772	25	320	32.27
2.673	41	321	33.50
2.500	2	400	35.89
2.424	24	410	37.05
2.356	2	411	38.15
2.294	10	331	39.24
2.237	4	420	40.29
2.184	8	421	41.31
2.133	9	332	42.33
2.043	10	422	44.30
2.001	2	430	45.27
1.961	19	510	46.25
1.926	2	511	47.15
1.857	7	520	49.00
1.827	2	521	49.88
1.741	6	522	52.52
1.716	2	530	53.34
1.691	2	531	54.18
1.668	2	600	55.01
1.645	6	610	55.84
1.623	15	611	56.66
1.582	4	620	58.26
1.563	10	621	59.06
1.544	7	541	59.86
1.526	3	533	60.62
1.508	2	622	61.40
1.492	8	630	62.17
1.475	5	631	62.96
1.444	4	444	64.50
1.429	3	632	65.24
1.415	2	710	65.97
1.400	2	711	66.74

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.387	1	640	67.47
1.374	2	720	68.21
1.3613	6	721	68.92
1.3366	3	642	70.38
1.3250	2	722	71.09
1.3136	3	730	71.80
1.3025	4	731	72.51
1.2807	3	650	73.95
1.2705	4	732	74.64
1.2413	3	810	76.71
1.2313	2	811	77.45
1.2224	1	733	78.12
1.2137	2	820	78.79
1.2049	3	821	79.48
1.1956	2	653	80.22
1.1790	3	822	81.59
1.1709	1	830	82.26
1.1630	4	831	82.95
1.1551	3	751	83.65
1.1473	1	662	84.33
1.1327	2	752	85.69
1.1117	2	841	87.72
1.1049	1	910	88.40
1.0982	2	911	89.08
1.0915	2	842	89.77
1.0853	1	920	90.43
1.0788	2	921	91.13
1.0666	2	664	92.47
1.0606	3	922	93.15
1.0548	2	930	93.82
1.0491	1	931	94.49
1.0376	1	852	95.87
1.0321	2	932	96.55
1.0161	2	940	98.59
1.0108	3	941	99.29
1.0057	1	933	99.98

Sample

The sample was prepared at NBS by melting an equimolar mixture of Rb_2SO_4 and $MnSO_4$.

Major impurities

0.01 -0.1 % each: Ag, Al, Cu, Na, and Sr

0.1 -1.0 % each: Cs

Color

Colorless

Optical data

Isotropic, N=1.590

Structure

Cubic, $P2_13$ (198), Z=4, langbeinite-type [Gattow and Zemann,1958]. The langbeinite structure was determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Gattow and Zemann [1958]--------	10.218 ±.004
NBS, sample at 25 °C----------	10.2147 ±.0001

Density

(calculated) 3.546 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.6$

References

Gattow,G. and J.Zemann(1958). Über Doppelsulfate vom Langbeinit-typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293, 233-240.

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$, Acta Cryst. 10, 409-413.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.901	2	111	15.00
4.170	6	211	21.29
3.613	6	220	24.62
3.405	2	221	26.15
3.230	100	310	27.59
3.081	17	311	28.96
2.950	1	222	30.27
2.833	3	320	31.55
2.731	50	321	32.76
2.554	2	400	35.11
2.479	12	410	36.21
2.344	4	331	38.37
2.284	2	420	39.41
2.228	3	421	40.45
2.179	7	332	41.40
2.086	15	422	43.34
2.043	2	430	44.30
2.004	22	510	45.21
1.967	2	511	46.11
1.898	7	520	47.89
1.866	2	521	48.76
1.805	1	440	50.52
1.778	5	522	51.33
1.752	2	530	52.16
1.727	2	531	52.99
1.703	1	600	53.79
1.679	4	610	54.60
1.658	15	611	55.37
1.615	5	620	56.96
1.595	7	621	57.74
1.576	6	541	58.50
1.557	2	533	59.29
1.540	2	622	60.02
1.523	6	630	60.76
1.506	5	631	61.52
1.474	3	444	62.99
1.459	3	632	63.72
1.445	2	710	64.43
1.431	1	711	65.15
1.417	2	640	65.85
1.403	2	720	66.60
1.390	6	721	67.30
1.365	3	642	68.71
1.353	2	722	69.43
1.341	2	730	70.13

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.3297	3	731	70.80
1.3080	2	650	72.16
1.2973	2	732	72.85
1.2771	1	800	74.19
1.2670	2	810	74.88
1.2572	2	811	75.57
1.2477	2	733	76.25
1.2389	1	820	76.89
1.2297	2	821	77.57
1.2208	2	653	78.24
1.2040	2	822	79.55
1.1954	1	830	80.24
1.1875	4	831	80.88
1.1793	2	751	81.56
1.1642	1	832	82.85
1.1563	2	752	83.54
1.1352	2	841	85.46
1.1278	1	910	86.15
1.1211	2	911	86.80
1.1143	2	842	87.46
1.1081	2	920	88.08
1.1013	3	921	88.76
1.0891	4	664	90.03
1.0826	4	922	90.72
1.0766	2	930	91.36
1.0708	2	931	92.00
1.0592	1	852	93.31
1.0536	3	932	93.96
1.0374	2	940	95.89
1.0319	2	941	96.57
1.0267	1	933	97.22
1.0216	2	10·0·0	97.88
1.0166	2	10·1·0	98.53
1.0116	<1	10·1·1	99.19
1.0017	1	10·2·0	100.53
0.9969	2	10·2·1	101.19
.9923	3	950	101.84
.9873	1	951	102.55
.9784	2	10·3·0	103.87
.9738	2	10·3·1	104.54
.9608	1	10·3·2	106.58
.9568	2	871	107.23
.9525	1	953	107.93
.9485	2	10·4·0	108.61
.9445	3	10·4·1	109.28
Plus 15	lines	to 0.8369	

Sample

The sample was prepared by fusion of RbCl and $SrCl_2$. The material was hygroscopic.

Color

Colorless

Optical data

Very low birefringence, $N \cong 1.550$; polysynthetic twinning.

Structure

Orthorhombic, Pnma (62), Z=4, distorted perovskite, by analogy with $RbCaCl_3$ and other ABX_3 compounds.

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C-------	7.924 ±.001	10.973 ±.002	7.631 ±.001

Density

(calculated) 2.797 g/cm³ at 25° C.

Internal standard Ag, a = 4.08641 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.49	11	101,020	16.14
4.91	10	111	18.06
3.962	30	200	22.42
3.885	100	121	22.87
3.818	35	002	23.28
3.521	4	201	25.27
3.435	6	102	25.92
3.350	8	211	26.59
3.296	10	031	27.03
3.282	12	112	27.15
3.211	7	220	27.76
3.134	6	022	28.46
3.043	12	131	29.33
2.960	11	221	30.17
2.910	9	122	30.70
2.744	80	040	32.60
2.686	10	230	33.33
2.666	10	212	33.59
2.534	4	231	35.40
2.497	11	301	35.94
2.455	12	222,141	36.57
2.435	15	311	36.89
2.273	20	321	39.62
2.256	20	240	39.92
2.227	25	042	40.48
2.217	40	123	40.67
2.141	4	203	42.17
2.109	3	051	42.84
2.062	6	331	43.88
1.980	9	400	45.78
1.941	20	242	46.75
1.907	11	004	47.65
1.863	6	420,251	48.85
1.848	7	233,341	49.28
1.758	4	402	51.96
1.737	12	323,412	52.65
1.715	5	252	53.37

Sample

The sample was prepared by slow evaporation at room temperature of an equimolar solution of Rb_2SO_4 and $ZnSO_4$.

Color

Colorless

Optical data

Biaxial (+) N_α=1.483, N_β=1.489, N_γ=1.497
2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2.
$Rb_2Zn(SO_4)_2 \cdot 6H_2O$ is a "Tutton Salt"[Tutton, 1893]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS sample at 25°C	9.185 ±.001	12.450 ±.002	6.242 ±.001	105°54.6′ ±.5′

Density

(calculated) 2.596 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.6

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.20	6	110	12.28
6.23	3	020	14.20
6.00	2	001	14.74
5.23	5	$\bar{1}11$	16.94
5.084	4	120	17.43
4.416	11	200	20.09
4.318	20	021	20.55
4.176	90	$\bar{1}11$	21.26
4.139	100	$\bar{2}01$	21.45
3.754	95	130	23.68
3.607	8	121,220	24.66
3.411	3	031	26.10
3.367	17	$\bar{1}31$	26.45
3.170	20	201	28.13
3.114	25	040	28.64
3.070	25	211	29.06
3.021	55	$\bar{1}12$,230	29.54
2.933	5	$\bar{2}31$,140	30.45
2.905	10	$\bar{3}11$	30.75
2.876	20	$\bar{2}02$	31.07
2.868	20	310	31.16
2.822	20	221	31.68
2.801	8	$\bar{2}12$	31.93
2.785	15	$\bar{1}22$	32.11
2.763	4	041	32.38
2.738	7	$\bar{1}41$	32.68
2.694	3	$\bar{3}21$	33.23
2.662	2	320	33.64
2.611	4	$\bar{2}22$	34.31
2.546	7	141,240	35.22
2.518	5	231	35.63
2.491	9	$\bar{1}32$,$\bar{2}41$	36.03
2.424	40	$\bar{3}31$,122	37.05
2.400	4	330	37.44
2.300	10	051	39.14
2.293	10	$\bar{3}22$	39.25
2.248	6	$\bar{4}11$	40.07
2.237	6	321	40.29
2.221	20	132,241	40.58
2.217	7	202	40.67

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.182	3	212	41.35
2.168	9	250	41.62
2.160	8	042	41.78
2.134	6	$\bar{2}51$	42.32
2.112	11	$\bar{2}42$	42.78
2.081	10	420	43.46
2.076	6	331,060	43.56
2.070	3	$\bar{4}02$	43.69
2.045	4	$\bar{2}03$	44.26
2.020	3	160,$\bar{2}13$	44.84
2.001	9	$\bar{4}31$,003	45.28
1.962	5	061	46.23
1.958	5	251	46.34
1.934	3	$\bar{3}42$	46.95
1.916	8	052	47.42
1.911	4	401	47.55
1.899	9	341	47.85
1.896	6	$\bar{3}13$	47.95
1.857	10	$\bar{1}33$	49.00
1.854	5	$\bar{2}61$	49.09
1.843	2	$\bar{2}33$	49.66
1.817	3	$\bar{5}11$	50.16
1.801	8	440	50.65
1.784	2	322	51.17
1.769	3	123	51.63
1.762	2	$\bar{5}21$	51.86
1.749	5	510	52.27
1.735	2	261,431	52.73
1.727	4	351,$\bar{1}62$	52.98
1.710	2	$\bar{2}43$	53.56
1.699	5	$\bar{1}71$,332,+	53.93
1.686	5	133	54.37
1.682	3	043,$\bar{2}62$,+	54.50
1.675	3	$\bar{4}23$	54.77
1.650	6	171,270	55.66
1.633	1	$\bar{3}43$,$\bar{2}71$	56.28
1.625	2	530	56.60
1.6091	5	$\bar{5}32$	57.20
1.5979	2	342	57.64

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. **117**, 334-357.

Tutton, A. E. (1893). Connection between the atomic weight of contained metals and the magnitude of the angles of crystals of isomorphous series. A study of the potassium, rubidium and cesium salts of the monoclinic series of double sulphates $R_2M(SO_4)_2 \cdot 6H_2O$, J. Chem. Soc. **63**, 337-423.

Rubidium Zinc Fluoride, $RbZnF_3$ (cubic)

Sample

The sample was prepared at NBS by adding a solution of $ZnCl_2$ to one of RbF in HF. The precipitate was washed in water and alcohol.

Major impurities

0.01 -0.1 % each: Al,Ca,Cr,Cu,Fe,and Pt

0.1 -1.0 % each: Ba and Mg

Color

Colorless

Optical data

Isotropic, N=1.508

Structure

Cubic, Pm3m (221), Z=1. Perovskite-type. Various distortions of the perovskite structure have been reported as shown in the lattice constant table. The NBS pattern was indexed with the smaller cubic cell; however diffraction peaks were not sharp which may indicate that there was a slight degree of distortion.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.13	<1	100	21.52
2.914	100	110	30.66
2.380	17	111	37.77
2.062	53	200	43.88
1.6829	38	211	54.48
1.4574	25	220	63.81
1.3033	13	310	72.46
1.2427	3	311	76.61
1.1899	6	222	80.68
1.1014	12	321	88.75
1.0307	2	400	96.76
0.9717	6	330	104.89
.9457	1	331	109.08
.9217	6	420	113.39
.8788	3	332	122.44
.8413	4	422	132.58
.8084	7	510	144.69

Lattice constants

	a(Å)	*c*(Å)
Ludekens and Welch [1952]	8.71*	8.03*
Klasens et al. [1953]	4.10**	
Schmitz-DuMont and Bornefeld [1956]	8.25*	
Crocket and Haendler [1960]	4.116	
NBS, sample at 25 °C	4.1215 ±.0001	

*from kX
**pseudocubic

Density

(calculated) 4.929 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 5.6

Additional patterns

1. PDF card 12-0039 [Schmitz-DuMont and Bornefeld]

References

Crocket,D.S. and H.M. Haendler(1960). Synthesis of fluorometallates in methanol. Some structure relationships, J.Am.Chem. Soc., 82,4158-4162.

Klasens, H. A., P. Zalm, and F. O. Huysman (1953). The manganese emission in ABF_3 compounds, Philips Res. Rept. 8,441-451.

Ludekens, W.L.W., and A.J.E. Welch (1952). Reactions between metal oxides and fluorides: some new double-fluoride structures of type ABF_3, Acta Cryst., 5, 841.

Schmitz-DuMont,O. and H. Bornefeld (1956). Die Systemreihe Alkalifluorid/Zinkfluorid, Z.Anorg.Allgem.Chem.,287,120-137.

Sample

The sample of thortveitite was synthesized hydrothermally by Jun Ito. A stoichiometric mixture of Sc_2O_3 and SiO_2 was heated to 700 °C at a pressure of 2 kilobars for 20 hours.

Color

Yellowish white

Optical data

Birefringent, N_α=1.745, N_γ=1.760

Structure

Monoclinic, C2/m (12), Z=2 [Gossner and Mussgnug, 1929]. Structure determined by [Zachariasen, 1930].

Density

(calculated) 3.394 g/cm³ at 25° C.

Additional patterns

1. PDF card 15-383 [Sakurai et al. 1962]
2. PDF card 15-798 [Toporov et al. 1962]
3. PDF card 19-1125 [Horne, 1966]
4. Sabina and Traill, [1960]
5. Sakurai et al. [1962] 2nd pattern

References

Gossner,B. and F. Mussgnug (1929). Beitrag zur Kenntnis des Thortveitites, Centr. Mineral., Geol. A, 1-5.

Horne,J.E.T.(1966). X-ray diffraction data for thortveitite, Bull. Geol. Surv. Gt. Brit. No.25, 97-99.

Sabina, A.P.and R.J.Traill (1960). Catalog of X-ray Diffraction Patterns and Specimen Mounts on File at the Geol. Surv. of Canada, Geol. Surv. Paper 60-4, 104.

Sakurai,K.,K.Nagashima, and A.Kato (1962). Thortveitite from Kobe,Omiya, Kyoto, Japan, Bull.Chem.Soc. Japan 35, 1776-1779.

Toporov, N. A. and V. A. Vasil'eva (1962). Equilibrium diagram of the scandium oxide-silica binary system, Russ.J.Inorg. Chem. 7, 1001-1005.

Zachariasen, W. H.(1930). The structure of thortveitite, $Sc_2Si_2O_7$, Z.Krist.73, 1-6.

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)	*β*(°)
Gossner et al. [1929]**---------	*6.57	8.60	4.75	103° 8′
Horne [1966]**----------	6.65	8.62	4.68	102°12′
	±.01	±.01	±.01	± 30′
NBS, sample at 25 °C----------	6.508	8.506	4.677	102°43′
	±.001	±.001	±.001	±1′

*as published
**natural mineral

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
5.09	15	110	17.40
4.57	7	001	19.41
4.257	3	020	20.85
3.131	100	111	28.48
3.114		021	28.64
2.926	47	$\bar{2}01$	30.53
2.588	15	130	34.63
2.543	13	220	35.26
2.373	3	201	37.89
2.279	2	002	39.50
2.236	2	$\bar{1}12$	40.29
2.169	18	131	41.60
2.126	3	040	42.48
2.084	10	$\bar{2}02$	43.39
2.073	8	221	43.62
2.043	16	$\bar{3}11$	44.29
2.010	1	022	45.06
1.957	1	112	46.35
1.927	5	041	47.12
1.870	14	$\bar{2}22$	48.64
1.794	2	$\bar{1}32$	50.85
1.737	3	311	52.62
1.720	4	$\bar{2}41, \bar{3}12$	53.21
1.696	7	330	54.01
1.690	10	$\bar{3}31$	54.22
1.685	9	202	54.40
1.640	19	132	56.02
1.587	5	400	58.08
1.519	6	151	60.96
1.507	9	$\bar{2}03$	61.49
1.493	6	$\bar{3}32$	62.14
1.489	5	$\bar{2}42$	62.32
1.462	2	$\bar{4}02$	63.59
1.418	7	060	65.83
1.391	3	113	67.24
1.366	7	$\bar{1}33$	68.64
1.335	3	421	70.46
1.323	5	$\bar{3}51$	71.20

Sample

A sample of SeO_2 from the Mallinckrodt Chemical Works was dried at 220 °C. The material was hygroscopic and the patterns were made with the sample enclosed in a dry mount.

Color

Colorless

Structure

Tetragonal, P4/mbc (135), Z=8, structure determined by McCullough [1937].

Lattice constants

	a(Å)	c(Å)
McCullough [1937]--------	8.370	5.061
Swanson and Tatge [1953]-	8.35	5.08
NBS, sample at 25 °C-----	8.3635 ±.0001	5.0635 ±.0002

Density

(calculated) 4.161 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.6$

Additional patterns

1. PDF card 4-429 [Swanson and Tatge,1953]

References

McCullough, J.D. (1937).The crystal structure of selenium dioxide, J. Am. Chem. Soc. 59, 789-794.

Swanson, H.E. and E. Tatge (1953). Standard X-ray Diffraction Powder Patterns, Natl.Bur.Std.U.S. Circ.539.Vol.I, 53-54.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.909	12	110	14.98
4.180	55	200	21.24
3.742	60	210	23.76
3.227	55	201	27.62
3.008	100	211	29.67
2.644	9	310	33.87
2.531	25	002	35.43
2.345	10	311	38.36
2.327	10	112	38.66
2.321	10	320	38.77
2.167	11	202	41.65
2.110	6	321	42.83
2.092	5	400	43.21
2.029	<1	410	44.63
1.972	2	330	45.98
1.933	18	401	46.98
1.883	14	411	48.30
1.870	5	420	48.65
1.829	14	312	49.82
1.754	10	421	52.09
1.710	11	322	53.53
1.673	1	430	54.83
1.640	2	510	56.03
1.589	1	431	58.00
1.566	5	203	58.94
1.5599	8	511	59.18
1.5528	8	520	59.48
1.5387	11	213	60.08
1.5041	3	422	61.61
1.4850	<1	521	62.49
1.4784	1	440	62.80
1.4340	1	530	64.98
1.4225	1	313	65.57
1.3956	2	432	67.00
1.3800	6	531	67.86
1.3748	9	610	68.15
1.3268	2	611	70.98
1.3237	5	522	71.17
1.3135	4	403	71.81
1.3064	1	540	72.26

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
1.2974	2	413	72.84
1.2798	1	621	74.01
1.2768	3	442	74.21
1.2646	4	541	75.05
1.2528	2	423	75.88
1.2105	5	631	79.04
1.2083	7	612	79.21
1.1826	1	550	81.29
1.1760	2	513	81.84
1.1608	2	542	83.15
1.1516	1	711	83.96
1.1112	2	324	87.77
1.0982	1	730	89.08
1.0929	2	533	89.63
1.0732	3	731	91.74
1.0709	2	650	91.99
1.0651	1	334	92.64
1.0546	<1	642	93.84
1.0475	2	651	94.67
1.0375	1	740	95.88
1.0331	<1	543	96.42
1.0238	<1	801	97.59
1.0162	<1	741	98.58
1.0143	1	820	98.83
1.0027	2	633	100.38
.9945	1	821	101.52
.9862	1	652	102.72
.9687	1	713	105.35
.9611	1	831	106.54
.9598	1	742	106.75
.9550	<1	751	107.53
.9457	1	315	109.07
.9415	1	822	109.79
.9351	1	840	110.92
.9314	3	614	111.59

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
.9236	1	910	113.02
.9204	2	733	113.62
.9113	1	405	115.40
.9089	2	544	115.88
.9073	2	760	116.20
.9041	1	653	116.85
.8930	1	921	119.22
.8815	1	930	121.82
.8772	1	842	122.83
.8732	1	851	123.81
.8684	<1	931	124.99
.8643	<1	554	126.06
.8539	1	762	128.85
.8492	1	940	130.20
.8466	<1	833	130.95
.8447	1	770	131.53
.8374	1	941	133.80
.8325	1	932	135.42
.8251	2	861	137.98
.8176	1	654	140.84
.8095	2	10·2·1	144.17
.8051	1	942	146.18
.8024	2	744	147.45
.8021	2	951	147.60
.8011	2	10·3·0	148.10
.7991	1	763	149.15

Sample
The sample was recrystallized from a water solution of reagent grade material from J.T.Baker Chemical Co.,Phillipsburg, N.J.

Color
Unground: deep orange
Ground: vivid orange

Optical data
Biaxial (+) N_α=1.660, N_β=1.698, N_γ=1.743
2V ≅ 90 °

Structure
Monoclinic, $P2_1/m$ (11), Z=4, [Campbell, 1956]

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
Campbell [1956]	12.6	10.5	6.05	94°54′
NBS, sample at 25°C	12.740 ±.001	10.778 ±.001	6.132 ±.001	95° 7′ ±1′

Density
(calculated) 2.360 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 0.8

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
8.20	5	110	10.78
6.34	5	200	13.95
5.70	20	$\bar{1}01$	15.54
5.47	25	210	16.19
5.40	80	020	16.40
5.31	20	101,011	16.69
5.041	20	$\bar{1}11$	17.58
4.957	10	120	17.88
4.772	20	111	18.58
4.607	10	$\bar{2}01$	19.25
4.239	40	$\bar{2}11$	20.94
4.105	10	220	21.63
4.042	10	021	21.97
3.924	85	211,$\bar{1}21$	22.64
3.786	25	121	23.48
3.632	5	$\bar{3}01$	24.49
3.502	30	$\bar{2}21$	25.41
3.444	5	$\bar{3}11$	25.85
3.321	20	221	26.82
3.175	20	400	28.08
3.041	100	410,$\bar{1}31$	29.35
3.013	15	$\bar{3}21$	29.62
2.976	10	131	30.00
2.937	5	012	30.41
2.927	10	$\bar{4}01$	30.52
2.911	25	102	30.69
2.852	10	$\bar{2}02$	31.34
2.834	40	$\bar{2}31$	31.54
2.821	30	$\bar{4}11$	31.69
2.812	40	112	31.80
2.760	10	$\bar{2}12$	32.41
2.735	25	231,420	32.72
2.716	10	401	32.95
2.696	20	040	33.20
2.642	3	$\bar{1}22$	33.90
2.635	5	140,411	34.00
2.589	10	$\bar{3}02$	34.62
2.582	10	212	34.71
2.560	5	122	35.02
2.516	5	$\bar{3}12$	35.65

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.471	5	510	36.32
2.447	3	331	36.69
2.438	5	$\bar{1}41$	36.84
2.428	5	421	37.00
2.403	5	141	37.39
2.384	5	222	37.70
2.362	5	$\bar{5}11$	38.07
2.332	3	$\bar{3}22$	38.57
2.320	2	312	38.78
2.305	2	$\bar{4}02$	39.05
2.271	10	340,241	39.66
2.263	5	132	39.80
2.233	3	$\bar{2}32$	40.35
2.223	3	511	40.55
2.209	3	$\bar{5}21$	40.81
2.168	2	431	41.63
2.115	5	600	42.72
2.100	5	$\bar{3}32$	43.04
2.095	5	521	43.14
2.074	<1	610,530	43.60
2.053	5	440	44.07
2.041	3	250	44.35
2.017	3	$\bar{1}51$	44.91
2.009	3	$\bar{5}31,\bar{5}12$	45.08
2.001	3	013	45.27
1.977	5	142	45.85
1.969	5	620	46.06
1.959	2	$\bar{2}42,\bar{2}13$	46.31
1.953	2	$\bar{2}51$	46.47
1.920	10	531,350,+	47.30
1.914	10	611,441	47.47
1.907	15	$\bar{1}23$	47.65
1.902	15	$\bar{3}03$	47.77
1.871	10	502	48.61
1.867	10	$\bar{2}23,\bar{3}42$	48.74
1.861	5	213,123	48.91
1.847	5	540	49.31
1.843	3	512	49.40
1.830	4	621	49.79
1.811	3	700,351	50.33

Internal standard W, a = 3.16516 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
1.800	5	$\bar{5}41$	50.66
1.796	5	060	50.80
1.783	5	342,$\bar{7}01$	51.20
1.775	5	$\bar{5}32$	51.43
1.763	3	$\bar{4}13$	51.82
1.758	5	$\bar{7}11,\bar{1}52$	51.96
1.752	3	$\bar{4}42$	52.15
1.732	10	152	52.81
1.720	10	$\bar{6}22,\bar{2}52$	53.22
1.692	2	$\bar{7}21$	54.17
1.673	10	$\bar{2}61,233$	54.83
1.663	5	640,$\bar{5}03$	55.20
1.657	10	$\bar{3}52$	55.41
1.642	5	550,$\bar{5}13$	55.94

Additional patterns

1. PDF card 1-0460 [Hanawalt et al.,1938].

References

Campbell, J.A. (1956). Note on the crystal structure of sodium dichromate dihydrate Acta Cryst. **9**, 192.

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-512.

Sample

J. Ito prepared the sample by heating lanthanum oxide and silicic acid with excess NaF. The crystals were removed from the molten NaF bath after several days.

*Exact analysis of percentages of Na and La is not known.

Color

Colorless

Optical data

Uniaxial (-) N_O=1.838, N_e=1.816

Structure

Hexagonal, $P6_3$ (173), Z=1, closely analogous to hydroxyapatite [Bowen and Dickens, 1968].

Lattice constants

	a(Å)	c(Å)
Bowen and Dickens [1968]	9.72	7.16
Ito [1968]	9.68	7.19
NBS, Sample at 25 °C	9.6890 ±.0002	7.1805 ±.0002

Density

(calculated) 4.971† g/cm³ at 25° C.

† assuming $Na_2La_8(SiO_4)_6F_2$

References

Bowen, J. S. and B. Dickens (1968). Private communication.

Ito, J. (1968). Private communication.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.195	24	200	21.16
4.013	25	111	22.13
3.622	4	201	24.56
3.594	32	002	24.75
3.300	41	102	27.00
3.172	31	210	28.11
2.901	100	211	30.80
2.883	70	112	30.99
2.798	28	300	31.96
2.727	3	202	32.81
2.378	2	212	37.80
2.328	9	310	38.64
2.296	3	221	39.20
2.207	4	302	40.85
2.146	15	113	42.08
2.098	7	400	43.08
2.080	3	203	43.47
2.009	21	222	45.10
1.953	16	312	46.45
1.926	6	320	47.16
1.910	36	213	47.56
1.860	17	321	48.93
1.831	17	410	49.76
1.811	22	402	50.33
1.795	19	004	50.82
1.774	2	411	51.47
1.697	1	322	53.98
1.683	1	114	54.48
1.679	1	500	54.63
1.668	1	313	55.01
1.651	3	204	55.62
1.6314	2	412	56.35
1.5858	5	420	58.12
1.5755	7	331	58.54
1.5626	10	214	59.07
1.5488	1	421	59.65
1.5206	8	502	60.87
1.5112	8	304	61.29
1.4997	8	323	61.81
1.4744	8	511	62.99

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.4728	9	332	63.07
1.4213	1	314	65.64
1.3896	1	512	67.33
1.3768	2	115	68.04
1.3732	2	601	68.25
1.3638	3	404	68.78
1.3546	1	431	69.31
1.3431	2	520	69.99
1.3389	3	333	70.24
1.3207	5	521	71.36
1.3128	3	324	71.85
1.3081	9	215	72.15
1.3031	6	602	72.47
1.2874	3	432	73.49
1.2817	10	414	73.88
1.2755	5	513	74.30
1.2597	8	611	75.39
1.2582	9	522	75.50
1.2356	1	225	77.13
1.2261	1	504	77.84
1.2112	4	440	78.98
1.1985	1	530	79.99
1.1967	2	006	80.13
1.1954	3	433	80.24
1.1888	3	424	80.77
1.1853	4	405,106	81.06
1.1824	1	531	81.30
1.1718	2	523	82.20
1.1635	1	620	82.91
1.1620	4	116	83.04
1.1541	2	514	83.74
1.1509	5	325,206	84.02
1.1473	2	442	84.35
1.1369	4	532	85.30
1.1286	2	613	86.08

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.1198	<1	216	86.92
1.1115	2	710	87.74
1.0758	1	524	91.45
1.0730	4	335,226	91.76
1.0644	4	425,316	92.72
1.0619	2	712	93.00
1.0489	1	800	94.51
1.0460	2	631	94.85
1.0420	3	614	95.33
1.0393	6	515,406	95.66
1.0290	3	542	96.93
1.0250	1	720	97.44
1.0141	3	632	98.85
1.0068	3	802	99.83
1.0040	5	444	100.21
0.9968	1	534	101.20
.9949	1	435	101.47
.9811	2	525	103.47
.9759	5	217	104.24
.9743	3	506	104.49
.9688	1	550	105.33
.9670	1	633	105.61
.9623	2	640	106.34
.9613	2	336	106.50
.9551	2	615,426	107.51
.9539	1	641	107.70
.9472	3	812	108.83
.9446	5	227	109.26

Sample source

Ito prepared the sample by heating neodymium oxide and silicic acid with an excess of NaF. The crystals were removed from the molten NaF bath after several days.

*Exact analysis of percentages of Na and Nd is not known.

Color

Unground- moderate purplish blue
Ground- pale purplish blue

Optical data

Uniaxial (-) N_O=1.884, N_e=1.860

Structure

Hexagonal, $P6_3$ (173), Z=1. Closely analogous to hydroxyapatite. [Bowen and Dickens, 1968]

Lattice constants

	a(Å)	c(Å)
Bowen and Dickens [1968]--	9.51	7.02
Ito [1968]----------	9.55	7.03
NBS, sample at 25 °C-----	9.5411 ±.0001	7.0331 ±.0002

Density

(calculated) 5.362‡ g/cm³ at 25° C.

‡assuming $Na_2Nd_8(SiO_4)_6F_2$

Reference intensity

$I/I_{corundum}$ = 3.2

References

Bowen, J.S. and B. Dickens (1968). Private communication.
Ito, J. (1968). Private communication.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.769	3	110	18.59
4.130	26	200	21.50
3.948	24	111	22.50
3.513	22	002	25.33
3.235	42	102	27.55
3.122	33	210	28.57
2.855	100	211	31.30
2.831	52	112	31.58
2.754	29	300	32.48
2.677	2	202	33.45
2.336	2	212	38.51
2.293	8	310	39.26
2.258	5	221	39.89
2.180	2	311	41.39
2.169	4	302	41.60
2.105	12	113	42.94
2.067	6	400	43.77
2.039	2	203	44.40
1.974	23	222	45.93
1.921	16	312	47.28
1.896	6	320	47.94
1.875	31	213	48.52
1.831	16	321	49.77
1.803	20	410	50.59
1.781	23	402	51.26
1.757	14	004	51.99
1.6690	1	322	54.97
1.6500	1	114	55.66
1.6177	3	204	56.87
1.6048	1	412	57.37
1.5614	4	420	59.12
1.5511	8	331	59.55
1.5322	8	214	60.36
1.5240	2	421	60.72
1.4960	10	502	61.98
1.4820	7	304	62.63
1.4743	8	323	63.00
1.4518	6	511	64.09
1.4487	8	332	64.24
1.4291	2	413	65.23
1.3948	2	314	67.04
1.3674	1	512	68.57
1.3490	2	115	69.64
1.3389	3	404	70.24
1.3338	3	431	70.55

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.3234	1	520	71.19
1.3162	3	333	71.64
1.3003	4	521,423	72.65
1.2893	2	324	73.37
1.2829	10	215,602	73.80
1.2673	2	432	74.86
1.2605	12	610	75.34
1.2586		414	75.47
1.2541	6	513	75.79
1.2401	6	611	76.80
1.2385	9	522	76.92
1.2117	1	225	78.94
1.2041	2	504	79.54
1.1991	1	315	79.94
1.1930	4	440	80.43
1.1862	2	612	80.99
1.1804	2	530	81.47
1.1756	2	441,433	81.87
1.1723	2	006	82.15
1.1676	3	424	82.56
1.1608	2	106	83.15
1.1522	3	523	83.91
1.1458	2	620	84.48
1.1381	4	116	85.19
1.1339	3	514	85.58
1.1307	4	621	85.88
1.1293	4	325,442	86.01
1.1190	4	532	87.00
1.1100	3	613	87.89
1.0974	1	216	89.16
1.0944	2	710	89.47
1.0894	1	622	89.99
1.0841	<1	604	90.56
1.0813	<1	711	90.86
1.0785	1	306	91.16
1.0751	1	434	91.53
1.0579	1	540	93.46
1.0543	3	533	93.87
1.0519	3	226	94.15
1.0453	3	425,712	94.94
1.0435	3	316	95.15
1.0409	1	630	95.47
1.0329	<1	800	96.45
1.0299	3	631	96.82
1.0244	4	614	97.52

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.0210	4	515	97.95
1.0195	3	406	98.14
1.0131	3	542	98.99
1.0095	3	720	99.47
0.9983	4	632	101.00
.9910	4	802	102.03
.9871	5	444	102.59
.9830	4	117,416	103.19
.9701	1	722	105.12
.9672	2	810	105.58
.9638	2	525	106.11
.9600	2	624	106.72
.9564	6	217	107.29
.9514	1	633	108.12
.9477	1	640	108.74
.9437	1	307,336	109.42
.9394	1	641	110.16
.9387	3	615	110.29
.9325	2	812	111.39
.9297	2	730	111.89
.9291	2	714	112.01
.9272	1	723	112.34
.9215	2	731	113.41
.9181	1	900	114.07
.9096	1	445	115.74
.9065	1	544	116.37
.9042	1	535	116.84
.8958	<1	634	118.61
.8942	3	821	118.95
.8926	2	606	119.30
.8905	1	804	119.76
.8877	3	327	120.40
.8838	<1	553	121.29
.8792	3	008	122.36
.8774	3	526	122.79
.8733	2	822	123.78
.8662	1	650	125.57
.8641	2	733	126.11
.8597	2	651	127.27
.8550	1	903	128.57
.8505	1	741	129.83
.8494	1	337	130.15

Sample source

Ito prepared the sample by heating praseodymium oxide and silicic acid with an excess of NaF. The crystals were removed from the molten NaF bath after several days.

*Exact analysis of percentages of Na and Pr is not known.

Color

Unground- brilliant yellow green
Ground- very light yellow green

Optical data

Uniaxial(-) N_o=1.874, N_e=1.855

Structure

Hexagonal, $P6_3$ (173) Z=1. Closely analogous to hydroxyapatite, [Bowen and Dickens,1968].

Lattice constants

	a(Å)	c(Å)
Bowen and Dickens [1968]--	9.58	7.05
Ito [1968]----------	9.60	7.09
NBS, sample at 25 °C-----	9.5828 ±.0002	7.0728 ±.0002

Density

(calculated) 5.207‡ g/cm³ at 25° C.

‡assuming $Na_2Pr_8(SiO_4)_6F_2$

Reference intensity

$I/I_{corundum}$ = 1.9

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.80	3	110	18.48
4.149	19	200	21.40
3.969	20	111	22.38
3.531	14	002	25.20
3.252	29	102	27.40
3.136	27	210	28.44
2.866	100	211	31.18
2.846	46	112	31.41
2.764	26	300	32.36
2.693	3	202	33.24
2.395	2	220	37.52
2.302	8	310	39.09
2.268	3	221,103	39.70
2.188	4	311	41.23
2.179	4	302	41.41
2.115	14	113	42.71
2.075	6	400	43.59
2.051	2	203	44.12
1.983	28	222	45.72
1.929	17	312	47.08
1.904	7	320	47.73
1.885	40	213	48.25
1.838	20	321	49.54
1.811	20	410	50.34
1.789	32	402	51.00
1.768	14	004	51.65
1.680	1	223	54.57
1.677	2	322	54.70
1.660	2	500,114	55.30
1.626	3	204	56.55
1.613	2	412	57.06
1.5681	6	420	58.84
1.5575	9	331,403	59.28
1.5403	10	214	60.01
1.5315	6	421	60.39
1.5023	12	502	61.69
1.4895	11	510,304	62.28
1.4810	10	323	62.68
1.4581	11	511	63.78
1.4556	11	332	63.90

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.4366	2	413	64.85
1.4334	2	422	65.01
1.4026	1	314	66.62
1.3738	1	512	68.21
1.3643	1	430	68.75
1.3574	2	601,503,+	69.15
1.3460	4	404	69.82
1.3399	3	431	70.18
1.3294	2	520	70.82
1.3224	4	333	71.25
1.3059	7	521,423	72.29
1.2956	4	324	72.96
1.2894	13	215	73.37
1.2729	2	432	74.48
1.2655	18	610,414	74.99
1.2600	6	513,305	75.37
1.2460	14	611	76.37
1.2439	8	522	76.52
1.2185	1	225	78.42
1.2105	2	504	79.04
1.1975	5	440	80.07
1.1913	2	612	80.57
1.1851	1	530,334	81.08
1.1809	3	441,433	81.43
1.1788	4	006	81.60
1.1735	5	424	82.05
1.1687	3	405	82.46
1.1671	2	106	82.60
1.1576	5	523	83.43
1.1508	3	620	84.03
1.1446	5	116	84.59
1.1397	4	514	85.04
1.1354	8	325	85.44
1.1240	7	532	86.52
1.1151	6	613,415	87.38
1.0995	4	710	88.95
1.0944	1	622	89.47
1.0864	1	711	90.31
1.0765	1	505	91.37
1.0625	2	540,524	92.93

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.0591	7	533,335	93.32
1.0575	6	226	93.51
1.0495	5	712,316	94.44
1.0375	2	800	95.88
1.0340	3	631,623	96.31
1.0290	5	614	96.93
1.0261	6	801,515	97.30
1.0250	6	406	97.44
1.0176	5	542	98.40
1.0139	1	720	98.88
1.0036	3	721	100.26
1.0027	5	632	100.39
0.9954	5	802	101.40
.9916	5	444	101.94
.9847	2	534	102.93
.9819	2	435,207	103.35
.9746	1	722	104.44
.9686	3	543,525	105.36
.9644	2	624	106.01
.9617	5	217	106.44
.9584	2	550	106.98
.9520	<1	640	108.02
.9485	3	336	108.61
.9432	3	615	109.51
.9365	3	812	110.67
.9334	4	730,714	111.23
.9310	3	227	111.65
.9258	2	731	112.62
.9220	1	900	113.32
.9193	1	642	113.84
.9085	2	535,407	115.97
.8980	2	821,813	118.13
.8971	2	606	118.32
.8947	3	804	118.84
.8925	5	327	119.32

References

Bowen,J.S.and B.Dickens(1968) Private communication.

Ito, Jun (1968). Private communication

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of Tl_2SO_4 and $CoSO_4$ in a 1:8 molar proportion. The first crystals formed were used.

Color

Unground: dark yellowish pink.
Ground: light pink

Optical data

Biaxial (-) N_α=1.599, N_β=1.613, N_γ=1.624
2V is medium large

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other "Tutton Salts" [Tutton, 1925]. The structure of a "Tutton Salt", $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.235 ±.001	12.442 ±.002	6.227 ±.001	106°24′ ±1′

Density

(calculated) 4.180 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.7$

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A.E. (1925). The monoclinic double sulphates containing thallium, thallium nickel and thallium cobalt sulphate, Proc.Roy.Soc. London,Ser.A 108, 240-261.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.213	22	110	12.26
6.219	1	020	14.23
5.977	11	001	14.81
5.388	16	011	16.44
5.089	26	120	17.41
4.429	2	200	20.03
4.310	9	021	20.59
4.225	35	$\bar{1}21$	21.01
4.154	100	111	21.37
3.952	5	$\bar{2}11$	22.48
3.757	55	130	23.66
3.611	2	220	24.63
3.463	1	$\bar{2}21$	25.70
3.368	6	$\bar{1}31$	26.44
3.159	16	201	28.23
3.112	25	040	28.66
3.059	15	211	29.17
3.019	46	131, $\bar{1}12$	29.56
2.991	3	002	29.85
2.935	8	140	30.43
2.922	14	$\bar{3}11$	30.57
2.907	14	012	30.73
2.881	23	$\bar{2}02$	31.01
2.817	10	221	31.74
2.781	12	$\bar{1}22$	32.16
2.756	7	041	32.44
2.737	8	$\bar{1}41$	32.69
2.669	6	320	33.55
2.617	2	$\bar{2}22$	34.24
2.560	1	112	35.03
2.542	1	141	35.28
2.513	5	231	35.70
2.490	15	$\bar{2}41, \bar{1}32$	36.04
2.433	27	$\bar{3}31, \bar{3}12$	36.91
2.412	11	122	37.25
2.406	10	330	37.34
2.302	16	$\bar{3}22$	39.10
2.298	15	$\bar{4}01$, 051	39.17
2.261	7	$\bar{4}11$	39.84
2.232	10	321	40.37

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.214	19	400,132	40.72
2.170	8	212,250	41.58
2.155	5	042,340	41.88
2.136	5	$\bar{2}51$	42.27
2.114	10	$\bar{2}42$	42.73
2.086	5	420	43.34
2.075	5	060	43.59
2.053	5	$\bar{4}12$	44.07
2.043	3	$\bar{1}13,\bar{2}03$	44.29
2.019	5	160,$\bar{2}13$	44.86
1.991	7	003	45.52
1.965	3	013,$\bar{1}23$	46.14
1.954	5	251,430	46.43
1.939	3	$\bar{3}42$	46.81
1.912	10	052	47.52
1.899	5	$\bar{3}13$	47.85
1.886	3	411	48.21
1.856	8	$\bar{2}61$	49.05
1.853	8	$\bar{1}33$	49.13
1.835	4	$\bar{3}23,312$	49.63
1.804	7	440	50.54
1.776	3	322	51.38
1.771	5	$\bar{5}21$	51.56
1.759	4	123	51.93
1.743	4	$\bar{3}33,170$	52.44
1.725	1	$\bar{1}62,351+$	53.03
1.704	3	520,071	53.74
1.692	5	332,$\bar{5}22$	54.16
1.6772	4	133,043	54.68
1.6489	5	270,171	55.70
1.6290	3	530	56.44
1.6179	4	$\bar{5}32$	56.86
1.5969	2	$\bar{4}52$	57.68
1.5801	3	143,$\bar{2}53$	58.35
1.5660	3	412	58.93
1.5554	3	080,053	59.37
1.5422	5	$\bar{2}14$	59.93
1.5299	4	$\bar{3}71$	60.46

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of Tl_2SO_4 and $CuSO_4$ in a 1:8 molar proportion. The first crystals formed were used.

Color

Unground: brilliant greenish blue
Ground: greenish white

Optical data

Biaxial, N_α=1.600, N_β=1.610, N_γ=1.620 2V is very large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2. Isostructural with other "Tutton" salts [Tutton, 1928]. The structure of a "Tutton" salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton, [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	9.268 ±.001	12.364 ±.001	6.216 ±.001	105°33.3′ ±.5′

Density

(calculated) 3.740 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.5$

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.22	26	110	12.24
5.98	13	001	14.79
5.394	20	011	16.42
5.084	22	120	17.43
4.467	4	200	19.86
4.302	10	021	20.63
4.197	100	111,210,+	21.15
4.153	70	$\bar{2}01$	21.38
3.940	13	$\bar{2}11$	22.55
3.742	64	130	23.76
3.623	3	220	24.55
3.450	1	$\bar{2}21$	25.80
3.399	2	031	26.20
3.350	8	$\bar{1}31$	26.59
3.195	28	201	27.90
3.091	38	040,211	28.86
3.024	36	230,131	29.51
3.008	37	$\bar{1}12$	29.67
2.920	22	140,$\bar{3}11$	30.59
2.910	19	012	30.70
2.894	13	310	30.87
2.868	26	$\bar{2}02$	31.16
2.837	11	221	31.51
2.795	3	$\bar{2}12$	32.00
2.773	16	$\bar{1}22$	32.25
2.746	7	041	32.58
2.721	9	$\bar{1}41$	32.89
2.682	10	320	33.38
2.603	4	$\bar{2}22$	34.43
2.523	4	231	35.55
2.477	18	$\bar{2}41,\bar{1}32$	36.23
2.428	37	$\bar{3}31$	36.99
2.421	35	032,$\bar{3}12$	37.11
2.412	15	330	37.24
2.375	2	311	37.85
2.304	7	$\bar{4}01$	39.06
2.291	16	$\bar{3}22$	39.29
2.286	17	051	39.39
2.265	8	$\bar{4}11$	39.77
2.254	11	321	39.96

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.232	8	400	40.38
2.221	23	241,$\bar{1}$32	40.58
2.191	2	212,$\bar{1}$42	41.17
2.162	9	250,151	41.74
2.154	5	$\bar{3}$41	41.91
2.124	8	$\bar{2}$51	42.53
2.117	6	$\bar{3}$32	42.67
2.102	16	$\bar{2}$42	43.00
2.061	4	060	43.89
2.047	6	$\bar{4}$12	44.20
2.041	6	$\bar{1}$13	44.34
2.009	6	$\bar{4}$31,$\bar{2}$13,+	45.08
2.005	6	142	45.19
1.996	10	003	45.40
1.964	2	$\bar{1}$23,430	46.19
1.959	4	232	46.32
1.939	3	$\bar{1}$61	46.81
1.928	4	401,$\bar{3}$42	47.10
1.907	12	052,411	47.64
1.890	5	$\bar{3}$13	48.11
1.850	10	$\bar{1}$33	49.21
1.846	9	$\bar{4}$41,$\bar{2}$61	49.33
1.827	5	$\bar{3}$23,$\bar{2}$33	49.86
1.809	10	440	50.40
1.794	2	322	50.86
1.775	6	$\bar{5}$21	51.45
1.769	10	123	51.64
1.766	6	510	51.71
1.747	2	431,$\bar{3}$52	52.33
1.737	4	$\bar{4}$03,$\bar{5}$12	52.65
1.733	5	170	52.79
1.715	4	$\bar{1}$62,520	53.38
1.705	7	332	53.70
1.687	4	$\bar{1}$71,$\bar{5}$22	54.34
1.684	6	$\bar{4}$51,133	54.43
1.674	4	$\bar{2}$62,$\bar{4}$23	54.80
1.649	2	213	55.71
1.644	4	270	55.89
1.641	6	171	56.00
1.638	6	530	56.10

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.626	2	$\bar{3}$43,$\bar{2}$71	56.55
1.614	4	$\bar{5}$32	57.01
1.590	3	$\bar{4}$52,$\bar{5}$41	57.95
1.582	4	412,$\bar{3}$62	58.27
1.5725	4	$\bar{2}$53	58.66
1.5502	2	$\bar{2}$04	59.59
1.5455	3	271,080,+	59.79
1.5378	4	$\bar{2}$14	60.12
1.5338	6	$\bar{1}$72,$\bar{1}$14	60.29
1.5229	5	180,$\bar{3}$71	60.77
1.5143	6	$\bar{4}$43,460	61.15
1.4995	5	$\bar{1}$24,$\bar{3}$14	61.82
1.4889	4	432,600	62.31
1.4732	2	313	63.05
1.4538	2	$\bar{5}$33	63.99
1.4344	4	$\bar{4}$04,063	64.96
1.4264	2	371	65.37
1.4179	3	442,$\bar{3}$34	65.81
1.4067	1	034,114	66.40

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 334-357.

Tutton, A. E.(1928). The hexahydrated double sulphates containing thallium, Proc. Roy. Soc. London, Ser. A 118, 367-392.

Sample

The sample was prepared by slowly evaporating a 1:8 mixture of molar solutions of Tl_2SO_4 and $MgSO_4$, and using the first crystals formed.

Color

Colorless

Optical data

Biaxial, N_α=1.570, N_β=1.588, N_γ=1.595, 2V is very large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2, isostructural with other "Tutton Salts" [Tutton, 1928]. The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
Hoffman [1932]	9.24	12.44	6.197	106° 30′
NBS, sample at 25°C	9.273 ±.001	12.472 ±.002	6.214 ±.001	106° 23′ ±1′

Density

(calculated) 3.532 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.6

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.24	50	110	12.22
6.24	2	020	14.19
5.95	19	001	14.87
5.37	19	011	16.48
5.10	33	120	17.37
4.44	2	200	19.97
4.30	8	021	20.62
4.227	53	$\bar{1}21$	21.00
4.162	100	111	21.33
3.957	8	$\bar{2}11$	22.45
3.764	66	130	23.62
3.467	2	$\bar{2}21$	25.67
3.369	6	$\bar{1}31$	26.43
3.164	25	201	28.18
3.117	40	040	28.61
3.065	21	211	29.11
3.025	47	230,131	29.50
3.010	39	$\bar{1}12$	29.65
2.982	5	002	29.94
2.931	26	$\bar{3}11$	30.47
2.897	21	012	30.84
2.882	35	$\bar{2}02$,310	31.00
2.820	8	221	31.70
2.808	7	$\bar{2}12$	31.84
2.777	18	$\bar{1}22$	32.21
2.742	11	$\bar{1}41$	32.63
2.678	13	320	33.43
2.614	1	$\bar{2}22$	34.27
2.555	4	112,240	35.09
2.517	7	231	35.64
2.499	21	$\bar{2}41$	35.91
2.488	20	$\bar{1}32$	36.07
2.442	35	$\bar{3}31$	36.77
2.412	18	330,122	37.25
2.302	24	051	39.10
2.270	10	$\bar{4}11$	39.68
2.239	11	321	40.24
2.222	25	241	40.57
2.205	9	202	40.86
2.171	9	212,151	41.57
2.155	3	042	41.88

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.141	8	$\bar{2}51$	42.18
2.116	10	$\bar{2}42$	42.70
2.096	3	420	43.12
2.079	2	222,060	43.50
2.058	5	$\bar{4}12$	43.97
2.039	3	$\bar{1}13$	44.39
2.024	3	160	44.75
2.018	4	$\bar{4}31$	44.89
1.987	6	003	45.62
1.960	7	251,430	46.29
1.955	6	$\bar{1}61$	46.40
1.942	3	$\bar{3}42$	46.74
1.913	9	401,052	47.48
1.898	4	$\bar{3}13$	47.90
1.862	4	$\bar{2}61$	48.88
1.851	5	$\bar{1}33$	49.17
1.835	5	$\bar{3}23$	49.63
1.811	8	440	50.35
1.801	2	242	50.64
1.778	5	$\bar{5}21$	51.35
1.760	5	$\bar{3}52$	51.91
1.757	5	123	51.99
1.746	7	$\bar{4}03$,170	52.35
1.724	1	$\bar{1}62$	53.00
1.711	1	$\bar{5}20$,$\bar{3}61$	53.52
1.695	5	332,451	54.07
1.676	3	133,043	54.72
1.651	6	252,171	55.61
1.635	4	213,343	56.20
1.622	3	$\bar{5}32$	56.72

References

Hoffman,W. (1931). Die Struktur der Tuttonschen Salze, Z. Krist, 78, 279-333.

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium and ammonium suflate hexahydrate, Z. Krist, 117, 344-357.

Tutton, A.E. (1928). The hexahydrated double sulphates containing thallium, Proc. Roy. Soc. London Ser. A 118 367-392.

Sample

The $Tl_2Mn_2(SO_4)_3$ was crystallized by evaporation at 90°C from a stoichiometric aqueous solution of Tl_2SO_4 and $MnSO_4$.

Major impurities

0.01 -0.1 % each: Al, Cu, and K

0.1 -1.0 % each: Mg

Color

Colorless

Optical data

Isotropic, N=1.722

Structure

Cubic, $P2_1/3$ (198), Z=4, langbeinite type, structure of langbeinite, $K_2Mg_2(SO_4)_3$, determined by Zemann and Zemann [1957].

Lattice constants

	a(Å)
Zemann and Zemann [1957]	10.223 ±.006
Gattow and Zemann [1958]	10.229 ±.004
NBS, sample at 25 °C	10.2236 ±.0002

Density

(calculated) 5.015 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.3$

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.90	27	111	15.01
5.110	2	200	17.34
4.574	12	210	19.39
4.172	18	211	21.28
3.613	22	220	24.62
3.407	12	221	26.13
3.232	100	310	27.58
3.082	18	311	28.95
2.951	1	222	30.26
2.834	22	320	31.54
2.731	58	321	32.76
2.479	24	410	36.20
2.409	1	411	37.29
2.356	7	331	38.34
2.286	2	420	39.38
2.231	8	421	40.39
2.180	8	332	41.39
2.087	17	422	43.31
2.045	3	430	44.26
2.005	33	510	45.18
1.968	2	511	46.09
1.899	9	520	47.87
1.867	3	521	48.74
1.807	1	440	50.46
1.779	4	522	51.31
1.754	1	530	52.10
1.729	1	531	52.92
1.704	1	600	53.76
1.681	4	610	54.56
1.659	17	611	55.34
1.617	5	620	56.91
1.596	12	621	57.70
1.577	9	541	58.46
1.559	3	533	59.21
1.541	<1	622	59.96
1.524	7	630	60.73
1.507	5	631	61.46
1.476	4	444	62.91
1.461	2	632	63.63
1.446	2	550	64.37

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.432	2	711	65.07
1.4179	1	640	65.81
1.4045	2	720	66.52
1.3912	7	721	67.24
1.3664	2	642	68.63
1.3541	1	722	69.34
1.3428	3	730	70.01
1.3310	3	731	70.72
1.3092	2	650	72.08
1.2983	3	732	72.78
1.2783	1	800	74.11
1.2682	3	810	74.80
1.2586	1	811	75.47
1.2493	2	733	76.13
1.2401	1	820	76.80
1.2308	4	821	77.49
1.2223	2	653	78.13
1.2050	2	822	79.47
1.1966	1	830	80.14
1.1885	5	831	80.80
1.1809	1	751	81.43
1.1729	1	662	82.10
1.1652	1	832	82.76
1.1576	2	752	83.43
1.1359	1	841	85.39
1.1290	1	910	86.04
1.1221	2	911	86.70
1.1158	1	842	87.31
1.1089	1	920	88.00
1.1025	2	921	88.64
1.0898	1	664	89.95
1.0837	3	922	90.60
1.0776	2	930	91.25
1.0717	<1	931	91.90
1.0601	1	852	93.21
1.0545	2	932	93.85
1.0381	1	940	95.80
1.0326	1	941	96.48
1.0275	1	933	97.12
1.0223	<1	10·0·0	97.78

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.0172	1	10·1·0	98.45
1.0122	<1	10·1·1	99.11
1.0025	1	10·2·0	100.42
0.9976	1	10·2·1	101.09
.9930	1	950	101.74
.9884	<1	951	102.40
.9838	1	10·2·2	103.06
.9792	1	10·3·0	103.74
.9747	1	10·3·1	104.42
.9617	1	10·3·2	106.44
.9576	<1	871	107.10
.9535	1	953	107.77
.9493	1	10·4·0	108.47
.9451	1	960	109.18
.9411	<1	10·3·3	109.86
.9333	1	10·4·2	111.25
.9294	<1	962	111.95
.9255	2	11·1·0	112.67
.9219	1	11·1·1	113.34
.9145	1	11·2·0	114.77
.9108	2	11·2·1	115.50
.9036	<1	880	116.95
.9001	2	11·2·2	117.69
.8932	1	11·3·1	119.16
.8898	1	10·4·4	119.91
.8864	1	964	120.69
.8831	2	11·3·2	121.44
.8766	2	10·6·0	122.98
.8735	<1	11·4·0	123.74
.8702	1	11·4·1	124.54
.8671	1	11·3·3	125.32
.8609	1	11·4·2	126.94
.8580	1	965	127.74
.8520	1	12·0·0	129.41
.8490	1	12·1·0	130.26

References

Gattow,G. and J. Zemann (1958). Über Doppelsulfate vom Langbeinit-Typ, $A_2^+B_2^{2+}(SO_4)_3$, Z. Anorg. Allgem. Chem. 293,233-240.

Zemann,A. and J. Zemann (1957). Die Kristallstruktur vom Langbeinit, $K_2Mg_2(SO_4)_3$ Acta Cryst. 10, 409-413.

Sample

The sample was prepared by slowly evaporating an equimolar solution of Tl_2SO_4 and $NiSO_4$.

Color

Unground: strong bluish green
Ground: very pale green

Optical data

Biaxial (-) N_α=1.602, N_β=1.615, N_γ=1.620
2V is large

Structure

Monoclinic, $P2_1/a$ (14), Z=2, isostructural with other "Tutton's salts" [Tutton, 1925]. The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25 °C	9.166 ±.001	12.392 ±.002	6.216 ±.001	106°20' ±1'

Density

(calculated) 3.763 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

References

Margulis, T. N. and D.H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium ammonium sulfate hexahydrate, Z. Krist. 117, 344-357.

Tutton, A.E.H. (1925). The monoclinic double sulfates containing thallium - thallium nickel and thallium cobalt sulphates. Proc. Roy. Soc.London Ser.A 118, 240-261.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.18	18	110	12.31
5.95	8	001	14.88
5.37	13	011	16.49
5.06	22	120	17.50
4.39	2	200	20.20
4.294	8	021	20.67
4.209	30	$\bar{1}21$	21.09
4.139	100	$111,\bar{2}01,+$	21.45
3.926	5	$\bar{2}11$	22.63
3.740	51	130	23.77
3.587	1	220,121	24.80
3.396	1	031	26.22
3.353	6	$\bar{1}31$	26.56
3.142	15	201	28.38
3.097	22	040	28.80
3.046	16	211	29.30
3.007	47	$131,\bar{1}12,+$	29.68
2.982	5	002	29.94
2.923	6	$\bar{2}31,140$	30.56
2.901	18	$\bar{3}11,012$	30.80
2.872	16	$\bar{2}02$	31.11
2.853	11	310	31.33
2.802	9	221	31.91
2.774	10	$\bar{1}22$	32.24
2.749	6	041	32.54
2.727	7	$\bar{1}41$	32.81
2.651	5	320	33.78
2.607	2	$\bar{2}22$	34.37
2.554	1	112	35.11
2.534	2	240,141	35.40
2.501	5	231	35.87
2.480	16	$\bar{1}32,\bar{2}41$	36.19
2.421	24	$\bar{3}31,\bar{3}12,+$	37.11
2.406	12	122	37.35
2.391	6	330	37.58
2.290	16	$\bar{3}22,051$	39.31
2.244	6	$\bar{4}11$	40.15
2.221	8	321	40.59
2.205	15	132,241	40.90
2.199	14	400,202	41.00
2.160	8	250,151	41.79
2.148	6	$\bar{3}41,042$	42.02
2.126	4	$\bar{2}51$	42.48
2.106	8	$\bar{2}42$	42.91
2.071	5	$420,222,+$	43.66

Internal standard Ag, a = 4.08641 Å CuKα_1 λ = 1.54056 Å; temp. 25 °C			
d (Å)	*I*	*hkl*	2θ(°)
2.065	5	060	43.80
2.042	5	$\bar{4}12,\bar{1}13,+$	44.33
2.012	4	$\bar{2}13,160$	45.02
1.997	3	$\bar{4}31,142$	45.37
1.988	5	003	45.60
1.963	2	$013,\bar{1}23,+$	46.22
1.945	5	$251,\bar{1}61$	46.66
1.929	2	$\bar{3}42$	47.07
1.906	7	$\bar{3}51,052$	47.68
1.893	4	023,350	48.02
1.887	4	341	48.18
1.875	2	$411,\bar{2}52$	48.50
1.849	9	$\bar{1}33,\bar{2}61$	49.24
1.829	3	$\bar{3}23,\bar{2}33$	49.81
1.793	8	440,242,+	50.89
1.770	2	$\bar{3}22$	51.59
1.757	5	$\bar{5}21,123$	52.00
1.742	4	$\bar{5}10$	52.50
1.737	5	$\bar{3}33,170$	52.66
1.724	3	431	53.09
1.720	3	$\bar{1}43,\bar{1}62$	53.22
1.692	3	$520,\bar{1}71$	54.15
1.687	5	332	54.34
1.680	4	$\bar{5}22,\bar{4}51$	54.59
1.673	5	$\bar{4}23,043,+$	54.82
1.642	5	270,171	55.95
1.618	2	530,441	56.84
1.608	4	$\bar{5}32$	57.25
1.589	2	$\bar{4}52,\bar{1}53$	58.01
1.576	3	$143,\bar{2}53$	58.53
1.558	3	511,412	59.24
1.551	3	$\bar{2}04,053$	59.57
1.538	5	$\bar{2}14,\bar{1}72$	60.10
1.526	3	$\bar{6}01,180$	60.64
1.523	4	$\bar{3}71,072,+$	60.78
1.516	5	$\bar{4}43,370,+$	61.07
1.505	4	$\bar{5}23,262,+$	61.56

Sample

The sample was prepared by slowly evaporating a 1:8 mixture of molar solutions of Tl_2SO_4 and $ZnSO_4$, and using the first crystals formed.

Color

Colorless

Optical data

Biaxial (-) N_α=1.592, N_β=1.610, N_γ=1.615
2V is large.

Structure

Monoclinic, $P2_1/a$ (14), Z=2, isostructural with other "Tutton's salts" [Tutton, 1910]. The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton [1962].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	9.219 ±.001	12.433 ±.002	6.2317 ±.0005	106°17.6′ ±.4′

Density

(calculated) 3.763 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 3.8

References

Margulis, T.N. and D. H. Templeton (1962). Crystal structure and hydrogen bonding of magnesium and ammonium sulfate hexahydrate, Z. Krist, 117, 344-357.

Tutton, A. E. H. (1910). The relation of thallium to the alkali metals: a study of thallium-zinc sulphate and selenate, Proc. Roy. Soc. London Ser.A 83 221-226.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
7.20	22	110	12.28
5.98	8	001	14.79
5.39	15	011	16.42
5.09	23	120	17.40
4.421	3	200	20.07
4.310	10	021	20.59
4.229	32	$\bar{1}21$	20.99
4.164	100	210,111,+	21.32
3.943	5	$\bar{2}11$	22.53
3.751	52	130	23.70
3.606	2	220,121	24.67
3.363	6	$\bar{1}31$	26.48
3.161	14	201	28.21
3.109	17	040	28.69
3.062	14	211	29.14
3.018	40	131,$\bar{1}12$	29.57
2.991	3	002	29.85
2.932	6	$\bar{2}31$,140	30.46
2.916	10	$\bar{3}11$	30.63
2.909	15	012	30.71
2.880	16	$\bar{2}02$	31.03
2.872	15	310	31.12
2.816	8	221	31.75
2.809	6	$\bar{2}12$	31.83
2.782	9	$\bar{1}22$	32.15
2.758	6	041	32.44
2.737	6	$\bar{1}41$	32.69
2.666	4	320	33.59
2.614	2	$\bar{2}22$	34.27
2.543	2	240,141	35.26
2.512	4	231	35.71
2.488	12	$\bar{2}41$,$\bar{1}32$	36.07
2.429	24	$\bar{3}31$,$\bar{3}12$	36.98
2.424	15	032	37.06
2.414	10	122	37.22
2.404	8	330	37.38
2.300	14	$\bar{3}22$	39.13
2.296	16	051,$\bar{4}01$	39.20
2.256	6	$\bar{4}11$	39.92
2.233	8	321	40.35

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.215	18	241,132	40.70
2.208	14	202,400	40.83
2.179	2	410	41.41
2.173	4	212	41.53
2.168	7	250,151	41.62
2.155	4	042	41.88
2.133	4	$\bar{2}51$	42.33
2.112	8	$\bar{2}42$	42.77
2.084	4	420	43.39
2.079	4	222,$\bar{4}02$	43.49
2.072	3	060,331	43.64
2.050	4	$\bar{4}12$	44.13
2.046	4	$\bar{1}13$,$\bar{2}03$	44.23
2.018	4	$\bar{2}13$,160	44.88
2.007	3	$\bar{4}31$	45.14
2.003	4	142	45.23
1.994	5	003	45.46
1.967	2	$\bar{1}23$	46.12
1.954	4	251	46.43
1.950	4	430,$\bar{1}61$	46.53
1.937	2	$\bar{3}42$	46.87
1.912	6	052	47.52
1.908	5	401	47.62
1.897	4	341,$\bar{3}13$,+	47.92
1.885	2	411	48.23
1.854	8	$\bar{2}61$,$\bar{1}33$	49.09
1.835	3	312,$\bar{3}23$,+	49.65
1.802	6	152,440	50.61
1.799	4	242	50.71
1.778	2	322	51.33
1.767	4	$\bar{5}21$	51.68
1.762	4	123	51.83
1.752	3	510	52.15
1.742	3	$\bar{3}33$,170	52.47
1.738	3	$\bar{5}12$	52.63
1.733	2	431,261	52.78
1.724	2	$\bar{1}62$,351,+	53.06
1.702	3	071,520	53.81
1.694	4	332	54.08
1.687	3	$\bar{4}51$	54.35

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
1.733	2	431,261	52.78
1.724	2	$\bar{1}62$,351,+	53.06
1.702	3	071,520	53.81
1.694	4	332	54.08
1.687	3	$\bar{4}51$	54.35
1.679	4	$\bar{4}23$,043	54.63
1.648	4	270,171	55.74
1.638	2	213	56.12
1.633	2	$\bar{3}43$,$\bar{2}71$	56.28
1.627	2	530	56.50
1.615	3	$\bar{5}32$	56.98
1.595	2	$\bar{4}52$	57.74
1.593	1	342,$\bar{1}53$	57.85
1.586	2	$\bar{5}41$	58.13
1.580	2	$\bar{2}53$,402	58.37
1.567	2	412,361	58.90
1.554	2	$\bar{2}04$,080	59.41
1.546	2	$\bar{5}13$	59.78
1.542	4	$\bar{2}14$,$\bar{1}72$	59.92
1.535	2	$\bar{6}01$,233	60.26
1.528	2	$\bar{3}71$,$\bar{5}42$	60.54
1.521	4	$\bar{4}43$,$\bar{3}53$	60.86
1.511	2	$\bar{5}23$,262,+	61.29
1.500	3	$\bar{1}81$,$\bar{6}02$	61.79
1.490	1	$\bar{6}21$	62.24
1.477	2	$\bar{5}31$	62.88
1.473	2	$\bar{3}24$	63.04
1.464	1	610	63.48
1.461	2	$\bar{3}13$	63.65
1.458	2	$\bar{5}33$,$\bar{6}22$,+	63.76
1.441	1	$\bar{4}04$,$\bar{6}31$	64.65
1.433	1	$\bar{5}52$	65.02
1.424	2	$\bar{3}34$	65.50

Sample

The sample was obtained from the National Lead Company, South Amboy, N.J.

Major impurities

No impurities greater than 0.001 percent

Color

Colorless

Structure

Tetragonal, $I4_1/amd$ (141), Z=4 [Huggins, 1926]

Lattice constants

	a(Å)	*c*(Å)
Swanson and Tatge (1953), sample at 26-27°C-------	3.783	9.51
NBS, sample at 25°C------	3.7852 ±.0001	9.5139 ±.0004

Density

(calculated) 3.893 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.3$

Polymorphism

Anatase and another mineral form, brookite (orthorhombic), are converted to a third mineral form, rutile (tetragonal), by heating to temperatures above 700 °C.

References

Huggins, M. L. (1926). The crystal structure of anatase and rutile, the tetragonal forms of TiO_2, Phys. Rev. 27, 638.

Swanson, H.E. and E. Tatge (1953) Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. U.S. Circ. 539, Vol. I, 46-47.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.515	100	101	25.32
2.431	9	103	36.95
2.378	22	004	37.80
2.332	9	112	38.57
1.892	33	200	48.05
1.6999	21	105	53.89
1.6665	19	211	55.06
1.4930	4	213	62.12
1.4808	13	204	62.69
1.3641	5	116	68.76
1.3378	5	220	70.31
1.2795	<1	107	74.03
1.2649	10	215	75.03
1.2509	3	301	76.02
1.1894	<1	008	80.72
1.1725	2	303	82.14
1.1664	5	224	82.66
1.1608	3	312	83.15
1.0600	1	217	93.22
1.0517	3	305	94.18
1.0436	3	321	95.14
1.0182	2	109	98.32
1.0070	2	208	99.80
.9967	1	323	101.22
.9555	4	316	107.45
.9464	3	400	108.96
.9246	<1	307	112.84
.9192	2	325	113.85
.9138	2	411	114.91
.8966	3	219,1·1·10	118.44
.8890	2	228	120.11
.8819	<1	413	121.73
.8793	2	404	122.34
.8464	2	420	131.02
.8308	<1	327	135.98
.8268	3	415	137.38
.8102	1	309	143.86
.7974	3	424	150.04
.7928	1	0·0·12	152.62

Sample

The sample was obtained from the National Lead Company, South Amboy, N.J.

Major impurities

No impurities greater than 0.001 percent

Color

Colorless

Structure

Tetragonal, $P4_2/mnm$ (136), Z=2 [Huggins, 1926]

Lattice constants

	a(Å)	c(Å)
Swanson and Tatge [1953]-	4.594	2.958
NBS, sample at 25 °C-----	4.5933 ±.0001	2.9592 ±.0001

Density

(calculated) 4.250 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.4$

Polymorphism

The two other mineral forms, anatase (tetragonal) and brookite (orthorhombic), are converted to rutile by heating to temperatures above 700 °C.

References

Huggins, M. L. (1926). The crystal structure of anatase and rutile, the tetragonal forms of TiO_2, Phys. Rev. **27**, 638.

Swanson, H.E. and E. Tatge (1953). Standard X-ray Diffraction Powder Patterns, Natl. Bur. Std. U.S. Circ. 539, I, 44-46.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.247	100	110	27.45
2.487	51	101	36.09
2.297	7	200	39.19
2.188	25	111	41.23
2.054	9	210	44.06
1.6874	60	211	54.32
1.6237	20	220	56.64
1.4797	9	002	62.74
1.4528	9	310	64.04
1.4243	1	221	65.48
1.3598	20	301	69.01
1.3465	11	112	69.79
1.3041	1	311	72.41
1.2441	3	202	76.51
1.2006	2	212	79.82
1.1702	5	321	82.33
1.1483	3	400	84.26
1.1143	2	410	87.46
1.0936	8	222	89.55
1.0827	4	330	90.71
1.0425	6	411	95.27
1.0364	6	312	96.01
1.0271	3	420	97.17
0.9703	1	421	105.09
.9644	2	103	106.01
.9438	1	113	109.40
.9072	4	402	116.22
.9009	4	510	117.53
.8892	8	212	120.06
.8774	8	431	122.79
.8738	8	332	123.66
.8437	6	422	131.83
.8292	8	303	136.55
.8196	12	521	140.05
.8120	2	440	143.09
.7877	2	530	155.85

Structure

Triclinic, $P\bar{1}$ (2), Z=1 [Jost et al., 1966]

Lattice parameters

a=7.25, b=5.70, c=4.67Å, α=99.8°, β=98.0°, γ=99.7° [ibid.]

Scattering factors

H°, O° [3.3.1A]
As° [3.3.1B]

Thermal parameters

Isotropic [Jost et al., 1966]

Density

(calculated) 3.45 g/cm³ [ibid.]

Scale factor

1.431×10^4

Reference

Jost,K.-H., H. Worzala, and E. Thilo (1966). Die Struktur des $As_2O_5 \cdot \frac{2}{3}H_2O$, Acta Cryst. **21**, 808-813.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
7.05	24	1 0 0	12.54
5.51	13	0 1 0	16.08
4.83	100	-1 1 0	18.36
4.53	4	0 0 1	19.58
3.98	4	1 1 0	22.34
3.54	40	1 0 1 +	25.10
3.43	39	-1 -1 1 +	25.98
3.28	2	-2 1 0	27.18
3.20	13	0 1 1 +	27.84
3.05	23	-2 0 1	29.24
2.754	6	0 2 0 +	32.48
2.736	5	2 1 0	32.70
2.712	1	-2 1 1	33.00
2.687	15	1 1 1	33.32
2.629	3	-2 -1 1	34.08
2.605	10	2 -1 1	34.40
2.593	10	0 -2 1	34.56
2.414	3	-2 2 0	37.22
2.353	1	3 0 0	38.22
2.336	2	-3 1 0	38.50
2.275	2	-1 0 2	39.58
2.268	2	0 0 2	39.70
2.260	6	0 -1 2	39.86
2.253	11	-3 0 1	39.98
2.229	1	-1 2 1	40.44

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
2.170	11	0 2 1	41.58
2.154	4	-3 1 1	41.90
2.082	2	-2 2 1	43.42
2.057	1	1 0 2	43.98
2.024	2	3 1 0	44.74
2.009	3	-1 1 2 +	45.10
1.9894	3	2 2 0	45.56
1.9545	1	3 0 1	46.42
1.9028	3	-2 1 2	47.76
1.8747	6	1 -2 2	48.52
1.8315	3	1 -3 1 +	49.74
1.8226	2	3 -2 1	50.00
1.7860	1	-4 1 0	51.10
1.7782	1	-2 3 0	51.34
1.7730	1	2 0 2	51.50
1.7647	2	4 0 0	51.76
1.7275	1	-4 1 1	52.96
1.7215	1	-1 -3 1	53.16
1.7131	2	-2 -2 2	53.44
1.7096	3	-3 -1 2	53.56
1.6996	1	2 -2 2	53.90
1.6967	3	1 3 0	54.00
1.6397	2	-1 3 1	56.04
1.6086	2	-3 3 0 +	57.22
1.5989	1	-2 3 1	57.60
1.5756	3	2 1 2	58.56
1.5633	2	-4 2 1	59.04
1.5594	1	3 -1 2	59.20
1.5341	1	-1 -3 2	60.28
1.5258	2	-4 0 2	60.64
1.5217	2	4 -2 1	60.82
1.5079	2	-3 -2 2 +	61.44
1.4986	2	-3 2 2	61.86
1.4869	3	1 2 2	62.40
1.4763	2	2 -3 2 +	62.90
1.4568	2	-4 -1 2	63.84
1.4395	2	-1 -2 3	64.70
1.4372	2	-5 1 0	64.82
1.4340	2	3 2 1	64.98
1.4277	1	1 0 3	65.30
1.4231	1	-2 -3 2	65.54
1.4101	1	1 -4 1 +	66.22
1.4034	1	-4 -2 1	66.58
1.3883	1	0 1 3	67.40
1.3847	1	-3 0 3	67.60
1.3768	2	0 4 0	68.04
1.3704	1	-5 2 0	68.40
1.3693	1	2 -4 1	68.46
1.3644	1	-3 -3 1	68.74
1.3603	1	4 -3 1	68.98
1.3507	1	2 -1 3	69.54

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.06	21	1 0 0	12.53
5.51	18	0 1 0	16.06
4.83	100	-1 1 0	18.36
4.53	4	0 0 1	19.57
3.98	4	1 1 0	22.33
3.55	42	1 0 1	25.10
3.53	4	2 0 0	25.21
3.43	42	-1 -1 1	25.98
3.40	2	1 -1 1	26.19
3.28	2	-2 1 0	27.17
3.22	1	-1 1 1	27.72
3.20	14	0 1 1	27.84
3.05	26	-2 0 1	29.24
2.755	3	-1 2 0	32.47
2.753	4	0 2 0	32.49
2.737	5	2 1 0	32.70
2.712	1	-2 1 1	33.00
2.686	17	1 1 1	33.32
2.629	4	-2 -1 1	34.08
2.605	12	2 -1 1	34.40
2.593	11	0 -2 1	34.57
2.414	3	-2 2 0	37.22
2.353	1	3 0 0	38.22
2.336	3	-3 1 0	38.50
2.275	2	-1 0 2	39.58
2.266	1	0 0 2	39.74
2.259	6	0 -1 2	39.86
2.253	10	-3 0 1	39.98
2.228	1	-1 2 1	40.44
2.170	14	0 2 1	41.58
2.155	5	-3 1 1	41.89
2.083	2	-2 2 1	43.41
2.057	1	1 0 2	43.99
2.024	3	3 1 0	44.73
2.009	3	-1 1 2	45.09
2.008	1	-2 -2 1	45.11
2.006	2	3 -1 1	45.15
1.9892	3	2 2 0	45.57
1.9546	1	3 0 1	46.42
1.9025	4	-2 1 2	47.77
1.8751	8	1 -2 2	48.51
1.8326	2	0 -3 1	49.71
1.8311	3	1 -3 1	49.75
1.8226	3	3 -2 1	50.00
1.7857	1	-4 1 0	51.11
1.7781	1	-2 3 0	51.34
1.7728	1	2 0 2	51.51
1.7646	3	4 0 0	51.77
1.7278	2	-4 1 1	52.95
1.7215	1	-1 -3 1	53.16

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7134	2	-2 -2 2	53.43
1.7097	4	-3 -1 2	53.56
1.7001	1	2 -2 2	53.86
1.6970	4	1 3 0	53.99
1.6395	3	-1 3 1	56.05
1.6091	2	-3 3 0	57.20
1.6080	1	-2 2 2	57.24
1.5992	1	-2 3 1	57.59
1.5748	4	2 1 2	58.57
1.5632	2	-4 2 1	59.05
1.5599	1	3 -1 2	59.18
1.5340	1	-1 -3 2	60.28
1.5260	2	-4 0 2	60.63
1.5213	2	4 -2 1	60.84
1.5081	1	-3 -2 2	61.43
1.5073	1	3 0 2	61.47
1.4987	2	-3 2 2	61.86
1.4872	4	1 2 2	62.39
1.4763	2	2 -3 2	62.90
1.4759	1	-2 -1 3	62.92
1.4654	1	1 -1 3	63.43
1.4569	2	-4 -1 2	63.84
1.4396	2	-1 -2 3	64.70
1.4372	2	-5 1 0	64.82
1.4341	2	3 2 1	64.98
1.4278	2	1 0 3	65.30
1.4228	1	-2 -3 2	65.56
1.4107	1	4 1 1	66.19
1.4099	1	1 -4 1	66.23
1.4033	1	-4 -2 1	66.58
1.3884	1	0 1 3	67.39
1.3848	1	-3 0 3	67.59
1.3767	2	0 4 0	68.04
1.3705	1	-5 2 0	68.39
1.3690	1	2 -4 1	68.48
1.3643	1	-3 -3 1	68.75
1.3601	1	4 -3 1	68.99
1.3506	2	2 -1 3	69.54
1.3413	1	2 3 1	70.10
1.3328	1	4 -1 2	70.61
1.3313	1	-5 -1 1	70.70
1.3140	1	2 -2 3	71.78
1.3054	1	0 3 2	72.33
1.3036	1	-5 0 2	72.44
1.2999	2	0 -3 3	72.68

Structure
Monoclinic, $P2_1/a$ (14), Z=4 [Brown,1966]

Lattice parameters
a=12.144, b=5.756, c=15.397Å, β=114°8′
(published value: c=15.396) [ibid.]

Scattering factors
H°, C°, N° [3.3.1A]

Thermal parameters
Anisotropic for carbon and oxygen, isotropic for hydrogen [Brown,1966]

Density
(calculated) 1.230 g/cm³

Scale factor
1.478 × 10^4

Additional patterns
1.PDF card 3-0172 [Socony-Vacuum, Paulsboro, N.J.]

Reference
Brown, C.J. (1966). A refinement of the crystal structure of azobenzene, Acta Cryst. 21, 146-152.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
14.06	6	0 0 1	6.28
7.02	36	0 0 2	12.60
5.60	13	2 0 -2	15.80
5.54	12	2 0 0	15.98
5.32	10	0 1 1	16.64
5.11	100	1 1 0 +	17.34
4.63	46	2 0 -3	19.16
4.56	70	2 0 1 +	19.46
4.53	95	1 1 1	19.56
4.45	77	0 1 2	19.92
4.18	24	2 1 -1	21.26
4.02	15	2 1 -2	22.12
3.99	5	2 1 0	22.24
3.83	50	1 1 -3	23.20
3.80	61	1 1 2	23.36
3.74	74	2 0 -4	23.80
3.68	66	2 0 2	24.16
3.63	14	0 1 3	24.48
3.61	9	2 1 -3	24.66
3.57	4	2 1 1	24.90

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.51	15	0 0 4	25.34
3.292	11	3 1 -2	27.06
3.285	8	3 1 -1	27.12
3.188	32	1 1 -4	27.96
3.168	7	1 1 3	28.14
3.134	5	2 1 -4 +	28.46
3.099	26	2 1 2	28.78
3.062	17	2 0 -5	29.14
3.035	4	4 0 -2	29.40
3.019	8	2 0 3	29.56
2.998	10	0 1 4	29.78
2.978	2	4 0 -3	29.98
2.870	3	3 1 -4	31.14
2.819	1	0 2 1	31.72
2.788	1	1 2 -1	32.08
2.703	4	2 1 -5	33.12
2.685	9	1 1 -5 +	33.34
2.679	8	1 2 1	33.42
2.674	8	2 1 3	33.48
2.664	6	0 2 2	33.62
2.644	2	4 1 -3	33.88
2.630	2	4 1 -1	34.06
2.600	3	2 2 -1	34.46
2.560	4	2 2 -2	35.02
2.538	2	3 1 2	35.34
2.503	3	1 2 2	35.84
2.497	3	4 1 0	35.94
2.452	1	0 2 3	36.62
2.444	1	2 2 -3	36.74
2.343	5	2 1 -6	38.38
2.336	5	3 2 -1 +	38.50
2.316	3	4 0 -6	38.86
2.279	2	4 0 2	39.50
2.271	2	3 2 0	39.66
2.267	1	2 2 2	39.72
2.258	2	3 1 3	39.90
2.183	1	5 1 -4	41.32
2.169	1	0 1 6	41.60
2.157	1	3 2 1	41.84
2.119	1	4 1 2	42.64
2.097	2	2 2 -5	43.10
2.089	1	4 2 -2	43.28
2.069	4	5 1 0	43.72
2.047	1	4 0 3	44.22
2.035	1	3 1 -7	44.48
2.017	1	3 2 2	44.90
2.010	4	3 1 4 +	45.06
1.9960	2	4 2 0	45.40
1.9665	3	5 1 -6	46.12
1.9529	2	6 0 -5	46.46

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.9364	1	6 0 -1	46.88
1.9279	1	4 1 3	47.10
1.9095	1	6 1 -3	47.58
1.9020	2	2 2 4	47.78
1.8908	3	1 2 -6	48.08
1.8842	2	1 2 5	48.26
1.8682	2	4 0 -8 +	48.70
1.8582	1	1 3 -2	48.98
1.8469	1	6 0 0	49.30
1.8399	2	4 0 4	49.50
1.8206	5	3 1 -8 +	50.06
1.8018	2	2 1 6	50.62
1.7945	1	1 3 2	50.84
1.7775	1	4 1 -8	51.36
1.7527	2	4 1 4	52.14
1.7465	1	2 2 -7	52.34
1.7197	1	3 2 4	53.22
1.7066	1	2 3 -4	53.66
1.6593	1	7 1 -4	55.32

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
14.05	5	0 0 1	6.28
7.03	32	0 0 2	12.59
5.61	12	2 0 -2	15.80
5.54	11	2 0 0	15.98
5.33	9	0 1 1	16.63
5.12	2	1 1 -1	17.30
5.11	100	1 1 0	17.35
4.63	44	2 0 -3	19.15
4.56	15	1 1 -2	19.45
4.56	46	2 0 1	19.46
4.53	82	1 1 1	19.56
4.45	78	0 1 2	19.92
4.18	25	2 1 -1	21.25
4.02	15	2 1 -2	22.12
3.99	3	2 1 0	22.25
3.83	49	1 1 -3	23.20
3.80	59	1 1 2	23.36
3.74	81	2 0 -4	23.79
3.68	70	2 0 2	24.16
3.63	13	0 1 3	24.48
3.61	7	2 1 -3	24.66
3.57	3	2 1 1	24.90
3.51	16	0 0 4	25.33
3.293	11	3 1 -2	27.05
3.283	2	3 1 -1	27.14
3.189	35	1 1 -4	27.96
3.168	6	1 1 3	28.15
3.135	3	2 1 -4	28.45
3.134	2	3 1 -3	28.45
3.101	30	2 1 2	28.77
3.062	19	2 0 -5	29.14
3.036	3	4 0 -2	29.40
3.020	8	2 0 3	29.56
2.999	11	0 1 4	29.77
2.977	1	4 0 -3	29.99
2.878	1	0 2 0	31.05
2.869	4	3 1 -4	31.15
2.819	1	0 2 1	31.71
2.788	1	1 2 -1	32.08
2.703	5	2 1 -5	33.11
2.686	1	1 2 -2	33.33
2.685	7	1 1 -5	33.34
2.685	2	4 1 -2	33.34
2.680	2	1 2 1	33.40
2.674	6	2 1 3	33.48
2.663	5	0 2 2	33.62
2.644	2	4 1 -3	33.87
2.631	3	4 1 -1	34.05
2.601	4	2 2 -1	34.46
2.560	4	2 2 -2	35.02

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.538	2	3 1 2	35.33
2.503	3	1 2 2	35.85
2.496	2	4 1 0	35.94
2.452	1	0 2 3	36.62
2.444	1	2 2 -3	36.74
2.344	5	2 1 -6	38.38
2.339	1	3 2 -2	38.45
2.336	3	3 2 -1	38.51
2.320	1	2 1 4	38.78
2.315	3	4 0 -6	38.87
2.279	1	4 0 2	39.51
2.270	1	3 2 0	39.67
2.267	1	2 2 2	39.73
2.257	2	3 1 3	39.91
2.184	2	5 1 -4	41.31
2.159	1	0 1 6	41.80
2.158	1	3 2 1	41.83
2.119	2	4 1 2	42.63
2.097	2	2 2 -5	43.10
2.089	1	4 2 -2	43.28
2.068	4	5 1 0	43.73
2.046	1	4 0 3	44.23
2.035	1	3 1 -7	44.47
2.017	1	3 2 2	44.90
2.010	4	3 1 4	45.07
2.008	1	6 0 -4	45.12

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.9960	3	4 2 0	45.40
1.9667	4	5 1 -6	46.12
1.9520	2	6 0 -5	46.46
1.9365	1	6 0 -1	46.88
1.9279	1	4 1 3	47.10
1.9092	1	6 1 -3	47.59
1.9023	2	2 2 4	47.77
1.8908	3	1 2 -6	48.08
1.8839	1	1 2 5	48.27
1.8686	2	4 0 -8	48.69
1.8686	1	6 0 -6	48.69
1.8671	1	3 2 3	48.73
1.8584	1	1 3 -2	48.97
1.8471	1	6 0 0	49.29
1.8401	2	4 0 4	49.49
1.8249	1	5 2 -4	49.94
1.8209	6	3 1 -8	50.05
1.8131	1	2 3 0	50.28
1.8016	2	2 1 6	50.63
1.7945	1	1 3 2	50.84
1.7773	1	4 1 -8	51.37
1.7527	2	4 1 4	52.14
1.7462	1	2 2 -7	52.35
1.7199	1	3 2 4	53.21
1.7069	1	2 3 -4	53.65
1.6594	1	7 1 -4	55.31

Structure

Cubic, $F\bar{4}3m$ (216), Z=4 [Harris and Yakel, 1966].

Lattice parameters

a=14.024±0.005 Å
(published value, 14.023 Å [ibid.])

Atomic positions

The parameters used are those in table 2 [ibid.]

Scattering factors

Be^{2+}, Ca^{2+} [Cromer and Waber, 1964]
O^{-} [3.3.1A]

Thermal parameters

Overall temperature factor=0.41679 [Harris and Yakel, 1966]

Density

(calculated) 2.64 g/cm^3 [ibid.]

Scale factor

85.75 × 10^4

Reference

Cromer, D.T. and J.T. Waber (1965). Scattering factors computed from relativistic Dirac-Slater wave functions, Acta Cryst. **18**, 104-109.

Harris, L. A. and H. L. Yakel (1966). The crystal structure of calcium beryllate, $Ca_{12}Be_{17}O_{29}$, Acta Cryst. 20, 295-301.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
8.10	100	1	1	1		10.92
7.01	26	2	0	0		12.62
4.96	34	2	2	0		17.88
4.23	6	3	1	1		21.00
4.05	3	2	2	2		21.94
3.51	40	4	0	0		25.38
3.218	13	3	3	1		27.70
3.136	15	4	2	0		28.44
2.863	21	4	2	2		31.22
2.699	19	3	3	3	+	33.16
2.479	39	4	4	0		36.20
2.371	3	5	3	1		37.92
2.338	38	4	4	2	+	38.48
2.217	3	6	2	0		40.66
2.139	1	5	3	3		42.22
2.114	4	6	2	2		42.74
2.024	51	4	4	4		44.74
1.9641	14	5	5	1	+	46.18
1.9450	4	6	4	0		46.66
1.8740	6	6	4	2		48.54
1.8261	9	7	3	1	+	49.90
1.7527	17	8	0	0		52.14
1.7131	7	7	3	3		53.44
1.7008	7	8	2	0		53.86
1.6527	18	8	2	2	+	55.56
1.6195	4	5	5	5	+	56.80
1.6086	3	6	6	2		57.22
1.5681	6	8	4	0		58.84
1.5392	1	9	1	1		60.06
1.5299	1	8	4	2		60.46
1.4951	1	6	6	4		62.02
1.4313	4	8	4	4		65.12
1.4094	1	7	7	1	+	66.26
1.4023	3	8	6	0		66.64
1.3750	2	8	6	2		68.14
1.3558	6	9	5	1	+	69.24
1.3493	2	6	6	6	+	69.62
1.3076	1	9	5	3		72.18
1.3020	3	10	4	0		72.54
1.2395	6	8	8	0		76.84
1.2253	2	9	5	5	+	77.90
1.2206	4	8	8	2	+	78.26
1.1895	1	9	7	3	+	80.72
1.1853	6	10	6	2		81.06
1.1687	1	12	0	0		82.46
1.1568	1	7	7	7	+	83.50
1.1376	2	12	2	2	+	85.24
1.1087	1	12	4	0		88.02
1.0984	1	9	9	1		89.06
1.0951	5	12	4	2	+	89.40

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.0820	1	10 8 2	90.78
1.0724	1	11 5 5	91.82
1.0694	2	10 6 6	92.16
1.0570	4	12 4 4	93.56
1.0481	1	11 7 3	94.60
1.0339	3	12 6 2	96.32
1.0255	1	13 3 3 +	97.38
1.0017	1	12 6 4	100.52
.9819	2	10 10 2 +	103.34
.9632	2	12 8 2 +	106.20
.9542	1	10 10 4 +	107.66
.9477	1	11 7 7 +	108.74
.9308	1	13 7 3 +	111.70
.9286	1	14 4 4	112.10
.9129	4	10 10 6 +	115.08
.8978	1	12 8 6	118.18
.8852	1	15 5 1 +	120.96
.8765	1	16 0 0	123.00
.8697	2	12 10 4 +	124.66
.8631	1	16 2 2 +	126.36
.8566	1	14 6 6	128.10
.8503	1	16 4 0	129.88
.8457	2	15 5 5 +	131.24
.8264	2	16 4 4 +	137.54
.8207	2	12 12 2 +	139.62
.8151	1	16 6 2 +	141.82
.8110	1	17 3 1 +	143.52
.8097	4	14 10 2 +	144.10
.8043	1	12 12 4	146.54
.8004	1	17 3 3 +	148.46
.7840	2	16 8 0	158.56
.7791	4	16 8 2 +	162.74

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
8.10	100	1 1 1	10.92
7.01	27	2 0 0	12.61
4.96	38	2 2 0	17.87
4.23	7	3 1 1	20.99
4.05	4	2 2 2	21.94
3.51	51	4 0 0	25.38
3.217	17	3 3 1	27.70
3.136	19	4 2 0	28.44
2.863	29	4 2 2	31.22
2.699	11	5 1 1	33.17
2.699	16	3 3 3	33.17
2.479	56	4 4 0	36.20
2.370	4	5 3 1	37.92
2.337	4	6 0 0	38.48
2.337	51	4 4 2	38.48
2.217	5	6 2 0	40.65
2.139	1	5 3 3	42.22
2.114	6	6 2 2	42.73
2.024	79	4 4 4	44.73
1.9637	3	7 1 1	46.19
1.9637	21	5 5 1	46.19
1.9448	5	6 4 0	46.67
1.8740	10	6 4 2	48.54
1.8258	11	7 3 1	49.91
1.8258	4	5 5 3	49.91
1.7530	29	8 0 0	52.13
1.7133	12	7 3 3	53.43
1.7007	12	8 2 0	53.86
1.6527	22	8 2 2	55.56
1.6527	8	6 6 0	55.56
1.6193	2	7 5 1	56.81
1.6193	4	5 5 5	56.81
1.6087	6	6 6 2	57.22
1.5679	11	8 4 0	58.85
1.5393	1	9 1 1	60.05
1.5301	2	8 4 2	60.45
1.4950	3	6 6 4	62.03
1.4313	8	8 4 4	65.12
1.4095	1	7 7 1	66.26
1.4095	1	7 5 5	66.26
1.4024	5	8 6 0	66.63
1.3752	3	8 6 2	68.13
1.3557	7	9 5 1	69.24
1.3557	4	7 7 3	69.24
1.3495	2	10 2 2	69.61
1.3495	2	6 6 6	69.61
1.3077	2	9 5 3	72.17
1.3021	6	10 4 0	72.54
1.2802	1	10 4 2	73.98
1.2645	1	7 7 5	75.06

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.2396	12	8	8	0	76.84
1.2253	1	11	3	1	77.90
1.2253	3	9	5	5	77.90
1.2206	6	8	8	2	78.26
1.2206	3	10	4	4	78.26
1.1895	1	11	3	3	80.72
1.1895	1	9	7	3	80.72
1.1852	12	10	6	2	81.07
1.1687	2	12	0	0	82.46
1.1567	1	11	5	1	83.51
1.1567	2	7	7	7	83.51
1.1375	4	12	2	2	85.25
1.1375	1	10	6	4	85.25
1.1087	2	12	4	0	88.02
1.0984	1	9	9	1	89.05
1.0951	7	12	4	2	89.40
1.0951	5	8	8	6	89.40
1.0820	2	10	8	2	90.78
1.0724	1	11	5	5	91.82
1.0693	4	10	6	6	92.17
1.0571	10	12	4	4	93.55
1.0482	2	11	7	3	94.59
1.0339	7	12	6	2	96.33
1.0255	2	13	3	3	97.37
1.0255	1	9	9	5	97.37
1.0121	1	8	8	8	99.12
1.0017	2	12	6	4	100.52
.9819	2	14	2	2	103.35
.9819	3	10	10	2	103.35
.9632	1	14	4	0	106.21
.9632	4	12	8	2	106.21
.9542	3	10	10	4	107.65
.9542	1	14	4	2	107.65
.9476	1	13	7	1	108.75
.9476	1	13	5	5	108.75
.9476	2	11	7	7	108.75
.9370	1	12	8	4	110.58
.9308	2	13	7	3	111.69
.9308	1	15	1	1	111.69
.9308	1	11	9	5	111.69
.9288	1	14	4	4	112.07
.9207	1	14	6	0	113.57
.9129	3	14	6	2	115.08
.9129	8	10	10	6	115.08
.8978	3	12	8	6	118.18
.8852	2	15	5	1	120.96
.8852	1	11	11	3	120.96
.8765	3	16	0	0	123.00
.8714	1	15	5	3	124.24
.8697	3	12	10	4	124.66

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
.8697	2	14	8	0	124.66
.8631	3	16	2	2	126.36
.8631	1	14	8	2	126.36
.8582	1	13	7	7	127.66
.8566	3	14	6	6	128.10
.8503	4	16	4	0	129.88
.8457	2	13	9	5	131.24
.8457	3	15	5	5	131.24
.8441	2	16	4	2	131.71
.8381	1	12	10	6	133.59
.8336	2	15	7	3	135.03
.8264	5	16	4	4	137.54
.8264	1	12	12	0	137.54
.8207	8	12	12	2	139.63
.8207	2	16	6	0	139.63
.8151	3	16	6	2	141.81
.8151	2	14	8	6	141.81
.8110	1	13	11	3	143.52
.8110	2	17	3	1	143.52
.8110	2	15	7	5	143.52
.8097	15	14	10	2	144.11
.8097	2	10	10	10	144.11
.8043	3	12	12	4	146.54
.8004	2	15	9	1	148.47
.8004	2	17	3	3	148.47
.7939	1	14	10	4	151.95
.7902	1	15	9	3	154.24
.7840	14	16	8	0	158.56
.7803	2	17	5	3	161.60
.7803	1	15	7	7	161.60
.7791	4	12	12	6	162.73
.7791	1	18	0	0	162.73
.7791	8	14	8	8	162.73
.7791	17	16	8	2	162.73

Structure

Cubic, Fd3m(227), Z=8 [Sands et al., 1959]

Lattice parameters

a=6.535±0.002Å [ibid.]

Scattering factors

Nb^0 [3.3.1B]

Be^0 [3.3.1A]

Thermal parameters

Isotropic [Sands et al., 1959]

Density

(calculated) 5.28 g/cm³ [ibid.]

Scale factor

11.88 × 10^4

Additional patterns

1. PDF 12-593 [Wright Air Development Center, Dayton, Ohio].

Reference

Sands, D.E., A. Zalkin, and O.H. Krikorian (1959). The crystal structures of $NbBe_2$ and $NbBe_3$, Acta Cryst. **12**, 461-464.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.5405 Å
3.773	100	1 1 1	23.56
2.311	78	2 2 0	38.94
1.9705	54	3 1 1	46.02
1.6337	8	4 0 0	56.26
1.4990	12	3 3 1	61.84
1.3339	18	4 2 2	70.54
1.2576	11	5 1 1 +	75.54
1.1552	6	4 4 0	83.64
1.1046	7	5 3 1	88.42
1.0332	7	6 2 0	96.40
0.9966	3	5 3 3	101.22
.9432	1	4 4 4	109.50
.9151	4	7 1 1 +	114.64
.8733	10	6 4 2	123.78
.8508	9	7 3 1 +	129.74
.8169	2	8 0 0	141.10
.7984	2	7 3 3	149.50

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.5405 Å
3.773	100	1 1 1	23.56
2.310	95	2 2 0	38.95
1.9704	68	3 1 1	46.02
1.6338	12	4 0 0	56.26
1.4992	19	3 3 1	61.83
1.3340	29	4 2 2	70.54
1.2577	14	5 1 1	75.53
1.2577	5	3 3 3	75.53
1.1552	11	4 4 0	83.63
1.1046	13	5 3 1	88.42
1.0333	14	6 2 0	96.40
0.9966	8	5 3 3	101.23
.9432	3	4 4 4	109.49
.9151	5	7 1 1	114.65
.9151	5	5 5 1	114.65
.8733	26	6 4 2	123.78
.8508	17	7 3 1	129.74
.8508	8	5 5 3	129.74
.8169	6	8 0 0	141.10
.7984	9	7 3 3	149.49

Structure
Orthorhombic, Fdd2 (43),Z=8 [Matković et al., 1966]

Lattice parameters
a=5.828±0.005, b=25.86±0.03, c=11.002±0.005Å [ibid.]

Scattering factors
O^{-1}, N° [3.3.1A]; Cd° [3.3.1B]

Thermal parameters
Isotropic.Cd(1) 2.2; O(2) 3.0; O(3) 5.5; O(4) 4.3; O(5) 4.7; O(6) 3.7; N(7) 3.1

Density
(calculated) 2.47 g/cm³ [Matković et al., 1966]

Scale factor
67.04×10^4

Additional patterns
1.PDF card 1-0242 [Hanawalt et al. 1938]

Reference

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-513.

Matković,B., B. Ribar, B.Zelenko, and S.W. Peterson (1966).Refinement of the structure of $Cd(NO_3)_2 \cdot 4H_2O$, Acta Crvst. 21, 719-725.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.46	28	0 4 0	13.70
5.06	100	0 2 2 +	17.52
4.42	46	1 3 1	20.08
3.65	24	1 5 1	24.38
3.393	3	0 6 2	26.24
3.232	5	0 8 0	27.58
3.083	8	1 1 3	28.94
3.002	13	1 7 1	29.74
2.921	15	1 3 3	30.58
2.843	1	2 2 0	31.44
2.751	4	0 0 4	32.52
2.662	16	1 5 3 +	33.64
2.574	8	2 0 2	34.82
2.531	2	0 4 4	35.44
2.525	3	2 2 2	35.52
2.509	4	1 9 1	35.76
2.414	6	2 6 0	37.22

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.393	8	2 4 2	37.56
2.377	3	1 7 3	37.82
2.340	9	0 10 2	38.44
2.211	1	2 6 2	40.78
2.155	1	0 12 0	41.88
2.139	7	1 11 1	42.22
2.108	5	1 9 3	42.86
2.095	5	0 8 4	43.14
2.052	2	1 1 5	44.10
2.014	9	2 8 2	44.98
2.002	5	1 3 5	45.26
1.9763	7	2 2 4	45.88
1.9341	3	2 10 0	46.94
1.9126	2	1 5 5	47.50
1.9080	3	3 1 1	47.62
1.8740	3	1 11 3	48.54
1.8675	4	3 3 1	48.72
1.8553	2	1 13 1	49.06
1.8145	6	2 6 4 +	50.24
1.7984	3	1 7 5	50.72
1.7938	3	3 5 1	50.86
1.7509	1	0 14 2	52.20
1.7131	2	3 1 3	53.44
1.6961	2	0 12 4	54.02
1.6874	1	0 6 6	54.32
1.6834	2	3 3 3	54.46
1.6749	2	1 13 3 +	54.76
1.6527	1	2 12 2	55.56
1.6348	1	1 15 1	56.22
1.6295	2	3 5 3	56.42
1.5824	1	2 10 4	58.26
1.5599	1	2 14 0	59.18
1.5566	1	3 7 3	59.32
1.5523	1	2 0 6	59.50
1.5485	1	1 11 5	59.66
1.5092	1	2 4 6	61.38
1.5070	1	1 15 3	61.48
1.4947	1	1 3 7 +	62.04
1.4840	1	3 11 1	62.54
1.4560	1	1 5 7	63.88
1.4540	1	3 1 5	63.98
1.4305	1	1 13 5	65.16
1.3993	2	2 8 6 +	66.80
1.3934	1	0 16 4	67.12
1.3901	1	0 18 2	67.30
1.3690	1	2 16 2	68.48
1.3386	1	4 6 2	70.26
1.2993	1	3 9 5 +	72.72
1.2376	1	4 10 2 +	76.98
1.1951	1	4 8 4 +	80.26

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.46	33	0 4 0	13.69
5.06	100	0 2 2	17.51
5.05	43	1 1 1	17.54
4.42	60	1 3 1	20.07
3.65	33	1 5 1	24.37
3.393	5	0 6 2	26.25
3.233	7	0 8 0	27.57
3.082	12	1 1 3	28.95
3.002	18	1 7 1	29.74
2.920	23	1 3 3	30.59
2.843	2	2 2 0	31.44
2.750	7	0 0 4	32.53
2.661	23	1 5 3	33.65
2.657	2	2 4 0	33.71
2.575	12	2 0 2	34.81
2.531	2	0 4 4	35.44
2.525	3	2 2 2	35.52
2.509	6	1 9 1	35.75
2.414	9	2 6 0	37.22
2.392	13	2 4 2	37.57
2.376	4	1 7 3	37.83
2.340	14	0 10 2	38.43
2.211	1	2 6 2	40.79
2.155	1	0 12 0	41.89
2.139	12	1 11 1	42.22
2.109	7	1 9 3	42.85
2.095	8	0 8 4	43.15
2.052	3	1 1 5	44.09
2.014	14	2 8 2	44.97
2.002	7	1 3 5	45.25
1.9767	12	2 2 4	45.87
1.9342	5	2 10 0	46.94
1.9126	3	1 5 5	47.50
1.9079	3	3 1 1	47.62
1.8740	5	1 11 3	48.54
1.8676	5	3 3 1	48.72
1.8556	3	1 13 1	49.05
1.8155	4	0 2 6	50.21
1.8143	8	2 6 4	50.24
1.7982	4	1 7 5	50.73
1.7943	3	3 5 1	50.85
1.7511	2	0 14 2	52.19
1.7129	4	3 1 3	53.45
1.6988	2	3 7 1	53.93
1.6963	3	0 12 4	54.01
1.6873	2	0 6 6	54.32
1.6836	3	3 3 3	54.45
1.6748	3	1 13 3	54.76
1.6734	1	1 9 5	54.81
1.6526	2	2 12 2	55.56

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6348	2	1 15 1	56.22
1.6293	2	3 5 3	56.43
1.5924	1	3 9 1	57.86
1.5822	2	2 10 4	58.27
1.5601	2	2 14 0	59.17
1.5568	1	3 7 3	59.31
1.5520	1	2 0 6	59.51
1.5487	1	1 11 5	59.65
1.5149	1	1 1 7	61.12
1.5091	2	2 4 6	61.38
1.5071	1	1 15 3	61.47
1.4956	2	0 10 6	61.99
1.4945	2	1 3 7	62.05
1.4838	2	3 11 1	62.55
1.4561	2	1 5 7	63.88
1.4540	1	3 1 5	63.98
1.4360	1	3 3 5	64.88
1.4305	2	1 13 5	65.16
1.4213	1	4 4 0	65.63
1.4037	1	1 7 7	66.56
1.4018	1	3 5 5	66.66
1.4001	1	4 2 2	66.75
1.3991	3	2 8 6	66.81
1.3935	1	0 16 4	67.12
1.3900	1	0 18 2	67.30
1.3789	1	3 13 1	67.92
1.3689	3	2 16 2	68.48
1.3570	1	2 14 4	69.17
1.3388	2	4 6 2	70.25
1.3283	1	4 8 0	70.89
1.3159	1	1 19 1	71.66
1.2996	1	3 13 3	72.70
1.2990	1	3 9 5	72.74
1.2886	1	2 18 0	73.42
1.2807	1	3 15 1	73.95
1.2655	1	0 8 8	74.99
1.2627	1	4 4 4	75.18
1.2594	1	2 12 6	75.42
1.2380	1	3 11 5	76.95
1.2380	1	2 2 8	76.95
1.2369	1	4 10 2	77.04
1.2234	1	1 17 5	78.04
1.1961	1	4 8 4	80.18
1.1949	1	2 6 8	80.27
1.1751	1	3 13 5	81.92
1.1669	1	2 18 4	82.62
1.1363	1	4 2 6	85.36
1.1200	1	4 14 2	86.90
1.1194	1	2 16 6	86.96

Structure
Tetragonal, $P4_1$ (76), Z=8 [Webb,1966]

Lattice parameters
a=6.684±0.006, c=24.145±0.015 Å [ibid.]
(published value, c=24.144±0.015 Å)

Scattering factors
Ca^{+2}, P^0 [3.3.1A]
O, an average of O^0 and O^- [3.3.1A]

Thermal parameters
Isotropic [Webb, 1966]

Density
(calculated) 3.128 g/cm³ [ibid.]

Scale factor
8.642×10^4

Additional patterns
1. PDF card 11-177 [St. Pierre, Dept. of Mines, Canada, Tech. paper No.2, p.105, 1953]

Reference
Webb,N.C.(1966). The crystal structure of β-$Ca_2P_2O_7$, Acta Cryst. **21**, 942-948.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.037	9	0 0 4	14.66
5.847	4	0 1 2	15.14
4.726	16	1 1 0	18.76
4.480	2	0 1 4	19.80
4.401	13	1 1 2	20.16
4.074	5	1 1 3	21.80
3.720	3	1 1 4	23.90
3.448	2	0 1 6	25.82
3.378	12	1 1 5	26.36
3.341	42	0 2 0	26.66
3.309	36	0 2 1	26.92
3.220	56	0 2 2	27.68
3.087	54	0 2 3	28.90
3.064	7	1 1 6 +	29.12
3.017	100	0 0 8	29.58
2.990	23	2 1 0 +	29.86
2.966	37	2 1 1 +	30.10
2.923	18	0 2 4	30.56
2.901	35	2 1 2 +	30.80
2.801	27	1 2 3 +	31.92

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.786	31	1 1 7	32.10
2.748	54	0 2 5	32.56
2.679	18	1 2 4 +	33.42
2.572	7	0 2 6	34.86
2.542	23	1 2 5 +	35.28
2.490	1	0 1 9	36.04
2.400	11	0 2 7 +	37.44
2.352	6	2 2 1	38.24
2.333	20	1 1 9	38.56
2.319	4	2 2 2	38.80
2.267	9	2 2 3 +	39.72
2.260	7	2 1 7	39.86
2.240	14	0 2 8	40.22
2.228	8	0 3 0	40.46
2.218	11	0 3 1	40.64
2.201	4	2 2 4	40.98
2.147	9	0 3 3 +	42.04
2.123	11	2 1 8 +	42.54
2.114	4	3 1 0 +	42.74
2.105	9	1 3 1 +	42.92
2.092	14	0 2 9 +	43.22
2.086	10	0 1 11	43.34
2.082	8	1 3 2 +	43.42
2.044	5	1 3 3 +	44.28
2.038	7	2 2 6	44.42
2.023	5	0 3 5	44.76
2.012	3	0 0 12	45.02
1.9960	18	1 2 9 +	45.40
1.9910	20	1 1 11	45.52
1.9569	9	0 2 10	46.36
1.9498	17	2 2 7	46.54
1.9364	5	1 3 5 +	46.88
1.8784	5	2 1 10	48.42
1.8711	6	3 1 6 +	48.62
1.8603	2	2 2 8	48.92
1.8539	13	3 2 0 +	49.10
1.8490	11	3 2 1	49.24
1.8343	12	0 2 11	49.66
1.8322	12	2 3 2 +	49.72
1.8064	2	2 3 3	50.48
1.8024	3	1 3 7 +	50.60
1.7925	2	0 3 8	50.90
1.7692	14	1 2 11 +	51.62
1.7312	5	2 3 5 +	52.84
1.7137	4	0 3 9	53.42
1.6886	4	2 2 10	54.28
1.6840	8	3 2 6 +	54.44
1.6693	3	0 1 14 +	54.96
1.6671	3	0 4 1	55.04
1.6604	4	1 3 9 +	55.28
1.6327	7	3 2 7 +	56.30
1.6232	6	0 2 13	56.66

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6200	7	1 1 14 +	56.78
1.6174	8	4 1 1 +	56.88
1.6066	6	4 1 2 +	57.30
1.5893	6	1 4 3 +	57.98
1.5794	7	3 2 8 +	58.38
1.5754	6	3 3 0	58.54
1.5720	4	3 3 1	58.68
1.5623	6	3 3 2 +	59.08
1.5434	2	0 4 6	59.88
1.5368	7	1 4 5 +	60.16
1.5322	6	2 2 12 +	60.36
1.5240	8	3 3 4 +	60.72
1.5092	1	0 0 16	61.38
1.5039	6	4 1 6 +	61.62
1.4934	6	0 3 12 +	62.10
1.4831	1	2 4 2	62.58
1.4671	5	4 1 7 +	63.34
1.4601	2	2 2 13	63.68
1.4572	4	3 1 12 +	63.82
1.4507	3	2 4 4 +	64.14
1.4328	1	3 3 7	65.04
1.4281	3	1 4 8 +	65.28
1.4162	4	2 3 11 +	65.90
1.4011	1	4 2 6	66.70
1.3963	2	3 3 8	66.96
1.3952	2	1 3 13	67.02
1.3930	2	2 2 14	67.14
1.3875	3	4 1 9 +	67.44
1.3750	1	0 2 16	68.14
1.3743	2	0 4 10	68.18
1.3715	2	2 4 7	68.34
1.3634	2	3 2 12	68.80
1.3599	3	1 1 17 +	69.00
1.3460	3	4 1 10 +	69.82
1.3393	1	4 2 8	70.22
1.3366	2	3 4 0 +	70.38
1.3304	3	2 2 15	70.76
1.3287	4	4 3 2 +	70.86
1.3194	3	3 3 10	71.44
1.3155	2	0 1 18	71.68
1.3117	2	1 5 0 +	71.92
1.3042	8	1 4 11 +	72.40
1.2904	1	1 1 18	73.30
1.2883	2	4 3 5 +	73.44
1.2805	2	1 3 15 +	73.96
1.2685	3	4 3 6 +	74.78
1.2653	2	1 5 5	75.00
1.2627	3	2 3 14 +	75.18
1.2495	2	0 3 16	76.12
1.2464	3	4 3 7 +	76.34
1.2404	1	3 3 12	76.78
1.2347	2	5 2 2	77.20

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.036	7	0 0 4	14.66
5.848	4	0 1 2	15.14
4.726	14	1 1 0	18.76
4.480	2	0 1 4	19.80
4.401	11	1 1 2	20.16
4.076	5	1 1 3	21.79
3.721	3	1 1 4	23.89
3.448	2	0 1 6	25.82
3.378	10	1 1 5	26.36
3.342	41	0 2 0	26.65
3.310	34	0 2 1	26.91
3.221	55	0 2 2	27.67
3.086	54	0 2 3	28.90
3.065	1	0 1 7	29.11
3.064	2	1 1 6	29.12
3.018	100	0 0 8	29.57
2.989	19	2 1 0	29.87
2.989	1	1 2 0	29.87
2.967	20	2 1 1	30.10
2.967	15	1 2 1	30.10
2.924	17	0 2 4	30.55
2.902	29	2 1 2	30.79
2.902	7	1 2 2	30.79
2.802	1	2 1 3	31.91
2.802	26	1 2 3	31.91
2.786	28	1 1 7	32.10
2.748	54	0 2 5	32.56
2.679	4	2 1 4	33.42
2.679	14	1 2 4	33.42
2.571	8	0 2 6	34.87
2.542	7	2 1 5	35.28
2.542	16	1 2 5	35.28
2.490	1	0 1 9	36.04
2.400	5	0 2 7	37.44
2.400	3	2 1 6	37.45
2.400	4	1 2 6	37.45
2.352	6	2 2 1	38.24
2.333	21	1 1 9	38.56
2.319	3	2 2 2	38.80
2.271	2	0 1 10	39.66
2.267	8	2 2 3	39.72
2.259	5	2 1 7	39.87
2.240	16	0 2 8	40.23
2.228	7	0 3 0	40.45
2.219	11	0 3 1	40.63
2.201	4	2 2 4	40.98
2.150	2	1 1 10	41.98
2.147	9	0 3 3	42.04
2.124	7	2 1 8	42.53
2.124	4	1 2 8	42.53
2.123	1	2 2 5	42.56
2.114	2	3 1 0	42.74

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.114	1	1 3 0	42.74
2.106	3	3 1 1	42.92
2.106	6	1 3 1	42.92
2.092	10	0 2 9	43.21
2.090	8	0 3 4	43.25
2.085	1	0 1 11	43.35
2.082	2	3 1 2	43.43
2.082	4	1 3 2	43.43
2.044	1	3 1 3	44.27
2.044	4	1 3 3	44.27
2.038	6	2 2 6	44.42
2.023	5	0 3 5	44.76
2.012	3	0 0 12	45.02
1.9966	10	1 2 9	45.39
1.9966	8	2 1 9	45.39
1.9949	3	1 3 4	45.43
1.9908	12	1 1 11	45.53
1.9571	9	0 2 10	46.35
1.9495	18	2 2 7	46.55
1.9363	2	3 1 5	46.88
1.9363	3	1 3 5	46.88
1.8783	5	2 1 10	48.42
1.8712	3	3 1 6	48.62
1.8712	2	1 3 6	48.62
1.8606	1	2 2 8	48.91
1.8538	9	3 2 0	49.10
1.8538	5	2 3 0	49.10
1.8513	2	1 1 12	49.17
1.8484	5	3 2 1	49.26
1.8347	11	0 2 11	49.65
1.8323	4	3 2 2	49.72
1.8323	6	2 3 2	49.72
1.8065	1	2 3 3	50.48
1.8022	1	3 1 7	50.61
1.8022	2	1 3 7	50.61
1.7925	2	0 3 8	50.90
1.7733	1	2 2 9	51.49
1.7721	2	3 2 4	51.53
1.7721	3	2 3 4	51.53
1.7692	6	2 1 11	51.62
1.7692	8	1 2 11	51.62
1.7313	1	3 1 8	52.84
1.7313	2	1 3 8	52.84
1.7307	2	3 2 5	52.86
1.7307	2	2 3 5	52.86
1.7238	1	0 2 12	53.08
1.7140	5	0 3 9	53.41
1.6889	4	2 2 10	54.27
1.6837	5	3 2 6	54.45
1.6837	4	2 3 6	54.45
1.6699	2	0 1 14	54.94
1.6692	1	1 2 12	54.96

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6670	2	0 4 1	55.04
1.6603	4	1 3 9	55.28
1.6603	1	3 1 9	55.28
1.6329	6	3 2 7	56.29
1.6329	2	2 3 7	56.29
1.6234	6	0 2 13	56.65
1.6211	2	1 4 0	56.74
1.6201	4	1 1 14	56.78
1.6175	5	4 1 1	56.88
1.6175	2	1 4 1	56.88
1.6083	3	2 2 11	57.23
1.6067	6	4 1 2	57.30
1.5904	1	1 3 10	57.94
1.5892	2	4 1 3	57.99
1.5892	5	1 4 3	57.99
1.5796	6	3 2 8	58.37
1.5791	1	0 4 5	58.39
1.5776	3	1 2 13	58.45
1.5754	3	3 3 0	58.54
1.5721	2	3 3 1	58.68
1.5636	3	0 3 11	59.03
1.5622	7	3 3 2	59.09
1.5432	2	0 4 6	59.89
1.5368	2	4 1 5	60.16
1.5368	7	1 4 5	60.16
1.5326	1	0 2 14	60.34
1.5320	3	2 2 12	60.37
1.5251	1	2 3 9	60.67
1.5244	6	3 3 4	60.70
1.5237	4	1 1 15	60.73
1.5225	1	1 3 11	60.79
1.5225	1	3 1 11	60.79
1.5091	1	0 0 16	61.39
1.5038	2	0 4 7	61.62
1.5037	4	4 1 6	61.63
1.5037	2	1 4 6	61.63
1.4938	1	1 2 14	62.08
1.4933	6	0 3 12	62.11
1.4917	1	4 2 1	62.18
1.4833	1	2 4 2	62.57
1.4671	4	4 1 7	63.34
1.4671	2	1 4 7	63.34
1.4670	2	3 3 6	63.35
1.4603	1	2 2 13	63.67
1.4573	4	3 1 12	63.82
1.4573	1	1 3 12	63.82
1.4508	2	2 4 4	64.14
1.4502	2	0 2 15	64.17
1.4330	1	3 3 7	65.03
1.4281	2	1 4 8	65.28
1.4278	1	4 2 5	65.30

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.4134	2	0 4 9	65.79
1.4103	2	3 2 11	65.90
1.4163	3	2 3 11	65.90
1.4011	1	4 2 6	66.70
1.3966	1	3 3 8	66.94
1.3952	1	1 3 13	67.02
1.3931	1	2 2 14	67.14
1.3893	1	0 1 17	67.35
1.3875	3	4 1 9	67.44
1.3875	1	1 4 9	67.44
1.3753	2	0 2 16	68.12
1.3740	1	0 4 10	68.19
1.3714	1	2 4 7	68.34
1.3634	2	3 2 12	68.80
1.3602	2	1 1 17	68.98
1.3585	2	3 3 9	69.08
1.3471	1	2 1 16	69.75
1.3459	3	4 1 10	69.82
1.3394	1	4 2 8	70.21
1.3368	2	3 4 0	70.37
1.3363	1	1 3 14	70.40
1.3304	3	2 2 15	70.76
1.3287	4	4 3 2	70.86
1.3287	1	3 4 2	70.86
1.3194	4	3 3 10	71.44
1.3152	1	0 1 18	71.70
1.3121	1	3 2 13	71.90
1.3108	1	1 5 0	71.98
1.3056	2	4 2 9	72.31
1.3056	1	2 4 9	72.31
1.3052	2	4 3 4	72.34
1.3048	1	0 3 15	72.36
1.3040	2	4 1 11	72.41
1.3040	8	1 4 11	72.41
1.2904	1	1 1 18	73.30
1.2883	1	4 3 5	73.44
1.2883	1	0 5 5	73.44
1.2806	1	1 3 15	73.95
1.2806	1	3 1 15	73.95
1.2686	2	4 3 6	74.77
1.2686	1	3 4 6	74.77
1.2651	1	1 5 5	75.02
1.2627	2	2 3 14	75.18
1.2627	1	3 2 14	75.18
1.2494	3	0 3 16	76.12
1.2465	1	4 3 7	76.34
1.2465	1	0 5 7	76.34
1.2404	1	3 3 12	76.77
1.2347	2	5 2 2	77.20
1.2282	2	3 1 16	77.68
1.2272	1	1 1 19	77.76

Structure

Orthorhombic, Pnma(62), Z=4 [Cromer et al., 1960]

Lattice parameters

a=8.112±0.001, b=5.102±0.001, c=10.162±0.005Å [ibid.]

Scattering factors

Ce^0, Cu^0 [3.3.1B]

Thermal parameters

Isotropic [Cromer et al., 1960]

Density

(calculated) 8.23 g/cm³ [ibid.]

Scale factor

13.17×10^4

Atomic positions

The positions used in these calculations are those in table 5 in the given reference.

Reference

Cromer, D.T., A.C. Larson, and R.B. Roof, Jr. (1960). The crystal structure of $CeCu_6$, Acta Cryst. 13, 913-918.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.5405 Å
6.338	3	1 0 1	13.96
4.304	7	1 0 2	20.62
4.055	3	2 0 0	21.90
3.973	9	1 1 1	22.36
3.767	1	2 0 1	23.60
3.171	12	2 0 2 +	28.12
3.031	9	2 1 1	29.44
2.822	29	0 1 3	31.68
2.693	1	2 1 2	33.24
2.665	8	1 1 3	33.60
2.614	2	3 0 1	34.28
2.552	35	0 2 0	35.14
2.425	50	1 0 4	37.04
2.386	15	3 0 2	37.66
2.367	9	1 2 1	37.98
2.326	100	3 1 1	38.68
2.317	97	2 1 3	38.84

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.5405 Å
2.279	27	0 2 2	39.50
2.194	15	1 2 2	41.10
2.159	34	2 2 0 +	41.80
2.112	29	2 2 1 +	42.78
1.9885	27	4 0 1 +	45.58
1.9835	47	2 1 4	45.70
1.9762	44	1 2 3	45.88
1.9713	42	1 0 5	46.00
1.9521	4	3 1 3	46.48
1.8841	4	4 1 0 +	48.26
1.8517	1	3 0 4	49.16
1.8391	2	1 1 5	49.52
1.8205	6	2 2 3	50.06
1.7672	1	4 1 2	51.68
1.7571	11	1 2 4	52.00
1.7403	3	4 0 3	52.54
1.7119	3	2 1 5	53.48
1.6581	2	1 0 6	55.36
1.6466	5	4 1 3 +	55.78
1.6428	4	1 3 1	55.92
1.6019	2	5 0 1	57.48
1.5628	5	2 0 6	59.06
1.5499	2	2 3 1	59.60
1.5480	2	3 1 5	59.68
1.5456	4	5 0 2	59.78
1.5285	4	5 1 1	60.52
1.5199	4	0 3 3	60.90
1.5154	3	4 2 2	61.10
1.4986	10	3 2 4	61.86
1.4942	6	1 3 3	62.06
1.4355	3	3 0 6	64.90
1.4254	15	3 3 1	65.42
1.4230	14	2 3 3	65.54
1.4108	5	0 2 6	66.18
1.3963	2	0 1 7	66.96
1.3900	6	1 2 6	67.30
1.3853	3	3 3 2	67.56
1.3817	9	4 1 5	67.76
1.3760	9	1 1 7	68.08
1.3672	6	5 0 4	68.58
1.3568	1	5 2 1	69.18
1.3520	2	6 0 0	69.46
1.3402	1	6 0 1	70.16
1.3346	6	2 3 4 +	70.50
1.3219	14	5 2 2	71.28
1.3067	2	6 0 2	72.24
1.3032	2	4 3 0	72.46
1.2998	3	4 0 6	72.68

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.5405$ Å
6.340	2	1 0 1	13.96
4.306	6	1 0 2	20.61
4.056	3	2 0 0	21.89
3.975	9	1 1 1	22.35
3.767	1	2 0 1	23.60
3.175	1	2 1 0	28.08
3.170	11	2 0 2	28.13
3.030	9	2 1 1	29.45
2.822	28	0 1 3	31.68
2.693	1	2 1 2	33.25
2.665	9	1 1 3	33.60
2.613	2	3 0 1	34.29
2.551	37	0 2 0	35.15
2.424	55	1 0 4	37.05
2.387	16	3 0 2	37.65
2.367	9	1 2 1	37.99
2.326	100	3 1 1	38.68
2.316	84	2 1 3	38.84
2.280	29	0 2 2	39.49
2.195	17	1 2 2	41.09
2.162	13	3 1 2	41.74
2.159	31	2 2 0	41.80
2.113	6	3 0 3	42.75
2.112	28	2 2 1	42.77
1.9888	25	4 0 1	45.57
1.9874	3	2 2 2	45.61
1.9836	35	2 1 4	45.70
1.9764	40	1 2 3	45.88
1.9715	24	1 0 5	46.00
1.9524	4	3 1 3	46.47
1.8846	3	4 1 0	48.25
1.8835	2	4 0 2	48.28
1.8515	1	3 0 4	49.17
1.8390	2	1 1 5	49.52
1.8209	7	2 2 3	50.05
1.7670	1	4 1 2	51.69
1.7574	14	1 2 4	51.99
1.7400	2	4 0 3	52.55
1.7117	4	2 1 5	53.48
1.6579	2	1 0 6	55.37
1.6469	6	4 1 3	55.77
1.6453	1	2 2 4	55.83
1.6426	1	1 3 1	55.93
1.6021	2	5 0 1	57.47
1.5629	6	2 0 6	59.06
1.5500	1	2 3 1	59.59
1.5481	2	3 1 5	59.68
1.5455	4	5 0 2	59.78
1.5285	5	5 1 1	60.52
1.5199	4	0 3 3	60.90

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.5405$ Å
1.5152	1	4 2 2	61.11
1.4984	13	3 2 4	61.87
1.4939	1	1 3 3	62.08
1.4354	4	3 0 6	64.91
1.4254	17	3 3 1	65.42
1.4232	15	2 3 3	65.53
1.4110	6	0 2 6	66.17
1.3963	2	0 1 7	66.96
1.3901	7	1 2 6	67.30
1.3851	2	3 3 2	67.57
1.3819	11	4 1 5	67.75
1.3761	12	1 1 7	68.08
1.3674	8	5 0 4	68.57
1.3567	1	5 2 1	69.18
1.3520	3	6 0 0	69.46
1.3402	2	6 0 1	70.16
1.3345	8	2 3 4	70.50
1.3327	1	2 2 6	70.62
1.3249	1	3 3 3	71.09
1.3219	19	5 2 2	71.28
1.3065	2	6 0 2	72.25
1.3031	1	4 3 0	72.47
1.3000	3	4 0 6	72.67
1.2755	13	0 4 0	74.30
1.2693	3	5 2 3	74.72
1.2680	1	5 0 5	74.81
1.2597	7	4 1 6	75.39
1.2557	1	6 0 3	75.67
1.2467	2	1 2 7	76.31
1.2417	1	2 3 5	76.68
1.2406	2	3 1 7	76.76
1.2186	2	1 1 8	78.40
1.2162	2	4 3 3	78.59
1.2048	2	2 2 7	79.48
1.1833	1	2 4 2	81.22
1.1748	1	3 3 5	81.94
1.1661	2	5 3 1	82.68
1.1629	11	6 2 2	82.96
1.1582	4	4 2 6	83.37
1.1371	1	0 2 8	85.28

Structure

Hexagonal, $P\bar{3}m1$ (164), Z=1 [Kaatz and Marcovich, 1966]

Lattice parameters

a=7.476±0.002, c=6.039±0.002 Å, [ibid.]

Scattering factors

Cl^- [Dawson, 1960]

Cs^+, Ce^{4+} [Thomas and Umeda, 1957]

All factors were corrected for anomalous dispersion using values given by Cromer [1965].

Thermal parameters

Isotropic [Kaatz and Marcovitch, 1966]

Density

(calculated)

3.52 g/cm³ [Kaatz and Marcovich, 1966]

Scale factor

10.44×10^4

Reference

Cromer, D.T. (1965). Anomalous dispersion corrections computed from self-consistent field relativistic Dirac-Slater wave functions, Acta Cryst. 18, 17-23.

Dawson,B.(1960). Atomic scattering factors from wave functions calculated by the poly-detor method:Cl,Cl^-,S and S^-, Acta Cryst. 13, 403-408.

Kaatz,T. and M.Marcovich (1966). The crystal structure of the compound Cs_2CeCl_6, Acta Cryst. 21, 1011.

Thomas, L. H. and K. Umeda (1957). Atomic scattering factors calculated from the TFD atomic model, J. Chem. Phys. 26,293-303.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
6.468	68	1 0 0	13.68
6.037	22	0 0 1	14.66
4.414	100	0 1 1 +	20.10
3.739	29	1 1 0	23.78
3.236	1	2 0 0	27.54
3.177	24	1 1 1	28.06
2.854	20	0 2 1 +	31.32
2.736	20	1 0 2 +	32.70
2.447	9	2 1 0	36.70
2.349	5	1 1 2	38.28
2.267	22	1 2 1 +	39.72
2.208	20	2 0 2 +	40.84
2.158	5	3 0 0	41.82
2.033	5	3 0 1 +	44.54
2.013	1	0 0 3	45.00
1.9225	6	1 0 3	47.24
1.9013	9	2 1 2 +	47.80
1.8689	10	2 2 0	48.68
1.7958	2	3 1 0	50.80
1.7853	3	2 2 1	51.12
1.7724	3	1 1 3	51.52
1.7559	2	0 3 2 +	52.04
1.7209	7	3 1 1	53.18
1.7096	2	2 0 3 +	53.56
1.5633	2	4 0 1 +	59.04
1.5547	4	2 1 3	59.40
1.5434	4	1 3 2 +	59.88
1.5096	1	0 0 4	61.36
1.4852	1	3 2 0	62.48
1.4721	1	0 3 3 +	63.10
1.4705	1	0 1 4	63.18
1.4423	3	2 3 1	64.56
1.4266	3	0 4 2 +	65.36
1.4128	2	4 1 0	66.08
1.4000	1	1 1 4	66.76
1.3757	2	1 4 1 +	68.10
1.3697	1	2 2 3	68.44
1.3399	2	1 3 3	70.18
1.3327	2	3 2 2 +	70.62
1.2850	1	1 2 4	73.66
1.2662	1	5 0 1	74.94
1.1991	1	2 4 1	79.94
1.1951	1	3 2 3	80.20
1.1873	1	0 1 5	80.90
1.1743	2	2 2 4	81.98
1.1419	1	1 5 1 +	84.84
1.1339	2	4 2 2 +	85.58
1.0829	1	1 2 5	90.68

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.474	64	1 0 0	13.67
6.039	20	0 0 1	14.66
4.416	2	1 0 1	20.09
4.416	100	0 1 1	20.09
3.738	31	1 1 0	23.78
3.237	1	2 0 0	27.53
3.178	28	1 1 1	28.05
2.853	5	2 0 1	31.33
2.853	19	0 2 1	31.33
2.737	11	0 1 2	32.70
2.737	13	1 0 2	32.70
2.447	11	2 1 0	36.69
2.349	6	1 1 2	38.29
2.268	1	2 1 1	39.71
2.268	27	1 2 1	39.71
2.208	13	2 0 2	40.83
2.208	12	0 2 2	40.83
2.158	6	3 0 0	41.82
2.032	4	3 0 1	44.55
2.032	3	0 3 1	44.55
2.013	2	0 0 3	45.00
1.9222	8	1 0 3	47.25
1.9011	7	2 1 2	47.80
1.9011	6	1 2 2	47.80
1.8690	13	2 2 0	48.68
1.7957	3	3 1 0	50.80
1.7854	4	2 2 1	51.12
1.7723	4	1 1 3	51.52
1.7558	1	0 3 2	52.04
1.7558	1	3 0 2	52.04
1.7212	10	3 1 1	53.17
1.7094	2	2 0 3	53.56
1.7094	1	0 2 3	53.56
1.5634	2	4 0 1	59.03
1.5634	1	0 4 1	59.03
1.5546	6	2 1 3	59.40
1.5434	3	3 1 2	59.88
1.5434	3	1 3 2	59.88
1.5097	2	0 0 4	61.35
1.4853	1	3 2 0	62.48
1.4720	1	3 0 3	63.10
1.4720	1	0 3 3	63.10
1.4703	1	0 1 4	63.19
1.4423	5	2 3 1	64.56
1.4266	2	0 4 2	65.36

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.4266	2	4 0 2	65.36
1.4128	2	4 1 0	66.08
1.3999	2	1 1 4	66.77
1.3757	1	4 1 1	68.10
1.3757	2	1 4 1	68.10
1.3697	2	2 2 3	68.44
1.3400	3	1 3 3	70.18
1.3328	2	3 2 2	70.61
1.3328	2	2 3 2	70.61
1.2849	1	1 2 4	73.67
1.2661	1	5 0 1	74.95
1.2460	1	3 3 0	76.37
1.2203	1	3 3 1	78.28
1.1992	1	2 4 1	79.93
1.1952	2	3 2 3	80.25
1.1873	1	0 1 5	80.90
1.1744	3	2 2 4	81.97
1.1564	1	4 1 3	83.53
1.1419	2	1 5 1	84.84
1.1340	2	4 2 2	85.57
1.1340	1	2 4 2	85.57
1.0831	1	1 2 5	90.67
1.0791	1	6 0 0	91.10
1.0482	1	3 4 1	94.59
1.0069	1	5 1 3	99.81
1.0022	1	3 1 5	100.46
.9744	1	6 1 1	104.47
.9409	1	4 3 3	109.89
.9371	1	2 3 5	110.57
.9345	1	4 4 0	111.03
.9142	1	5 3 1	114.81
.8864	1	1 6 3	120.67
.8606	1	2 6 2	127.03
.8404	1	3 5 3	132.84
.8377	1	1 5 5	133.71
.8213	1	4 5 1	139.41
.8136	1	2 1 7	142.42
.7985	1	3 4 5	149.42
.7946	2	4 4 4	151.58
.7843	1	7 2 1	158.32

Structure

Orthorhombic, Pmcn (62), Z=4 [Carpenter, 1966].

Lattice parameters

a=6.634, b=9.567, c=10.958Å [ibid.]

Scattering factors

Cs°, I°, Br° [3.3.1B]

Thermal parameters

Isotropic: Cs 3.22; Br 2.31; I(2) 2.08; I(3) 2.80

Density

(calculated) 4.456 g/cm³ [Carpenter,1966]

Scale factor

40.80 × 10^4

Reference

Carpenter, G.B. (1966). The crystal structure of CsI_2Br, Acta Cryst. 20, 330-334.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.45	10	1 1 0	16.24
4.88	2	1 1 1	18.16
4.78	6	0 2 0	18.54
4.76	4	0 1 2	18.64
4.38	2	0 2 1	20.24
4.22	6	1 0 2	21.02
3.86	31	1 1 2	23.00
3.66	44	1 2 1	24.32
3.60	12	0 2 2	24.68
3.411	6	0 1 3	26.10
3.316	69	2 0 0	26.86
3.166	100	1 2 2	28.16
3.033	5	1 1 3	29.42
2.873	11	1 3 0	31.10
2.779	2	1 3 1	32.18
2.756	8	0 3 2	32.46
2.740	14	0 0 4	32.66
2.731	9	2 2 0	32.76
2.659	25	1 2 3	33.68
2.633	8	0 1 4	34.02
2.532	7	1 0 4	35.42
2.440	7	2 2 2	36.80
2.391	2	0 4 0	37.58
2.378	7	2 1 3 +	37.80
2.336	10	0 4 1	38.50
2.259	3	1 3 3	39.88
2.204	3	1 4 1	40.92
2.192	1	0 4 2	41.14
2.136	4	0 1 5	42.28
2.120	7	2 3 2	42.62

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.112	11	2 0 4	42.78
2.078	4	0 3 4	43.52
2.062	5	2 1 4	43.86
2.005	3	3 1 2	45.18
2.001	4	0 4 3	45.28
1.9746	5	3 2 1	45.92
1.9403	2	2 4 0	46.78
1.9325	3	2 2 4	46.98
1.9156	8	1 4 3	47.42
1.9103	12	2 4 1	47.56
1.8849	15	3 2 2	48.24
1.8560	1	3 1 3	49.04
1.8385	2	1 5 0	49.54
1.8286	1	2 4 2	49.82
1.8172	2	3 3 0	50.16
1.8131	2	1 5 1	50.28
1.8064	1	0 5 2	50.48
1.7958	4	2 1 5 +	50.80
1.7597	7	3 2 3 +	51.92
1.7428	3	1 3 5 +	52.46
1.7385	6	1 4 4	52.60
1.7318	6	1 1 6	52.82
1.7209	2	3 0 4	53.18
1.7131	3	2 4 3	53.44
1.7060	3	0 2 6	53.68
1.6587	5	4 0 0	55.34
1.6386	1	2 5 1	56.08
1.6159	1	0 4 5	56.94
1.6060	1	3 4 1	57.32
1.5863	1	2 5 2	58.10
1.5779	3	0 6 1 +	58.44
1.5350	2	1 6 1	60.24
1.5267	1	1 5 4	60.60
1.5172	2	2 2 6	61.02
1.5065	1	4 2 2	61.50
1.5048	1	1 1 7	61.58
1.4835	2	3 4 3	62.56
1.4524	2	2 4 5 +	64.06
1.4479	1	3 5 0	64.28
1.4250	2	2 6 1	65.44
1.4212	2	4 3 2	65.64
1.4185	2	4 0 4	65.78
1.4082	1	3 0 6	66.32
1.4034	1	4 1 4	66.58
1.3967	2	3 4 4	66.94
1.3934	2	3 1 6	67.12
1.3746	1	1 3 7	68.16
1.3603	1	4 2 4	68.98
1.3524	2	4 4 1	69.44
1.3493	2	1 6 4	69.62
1.3297	1	2 4 6	70.80

Calculated Pattern *(Integrated)*						Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å	*d* (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
5.45	9	1	1	0	16.25	1.8064	1	0	5	2	50.48
4.88	1	1	1	1	18.16	1.7960	5	2	1	5	50.79
4.78	5	0	2	0	18.53	1.7939	1	0	1	6	50.86
4.75	3	0	1	2	18.65	1.7610	4	2	3	4	51.88
4.38	2	0	2	1	20.24	1.7608	2	1	0	6	51.88
4.22	6	1	0	2	21.01	1.7591	6	3	2	3	51.94
3.86	29	1	1	2	22.99	1.7429	1	1	5	2	52.46
3.66	42	1	2	1	24.32	1.7427	2	1	3	5	52.46
3.60	12	0	2	2	24.69	1.7387	6	1	4	4	52.59
3.412	6	0	1	3	26.09	1.7317	6	1	1	6	52.82
3.317	68	2	0	0	26.86	1.7207	2	3	0	4	53.19
3.166	100	1	2	2	28.16	1.7135	3	2	4	3	53.43
3.034	5	1	1	3	29.41	1.7062	3	0	2	6	53.67
2.874	12	1	3	0	31.09	1.6585	6	4	0	0	55.35
2.780	2	1	3	1	32.17	1.6386	1	2	5	1	56.07
2.756	8	0	3	2	32.46	1.6270	1	3	3	3	56.52
2.740	14	0	0	4	32.66	1.6156	1	0	4	5	56.94
2.726	2	2	2	0	32.83	1.6061	1	3	4	1	57.32
2.720	1	2	1	2	32.90	1.5864	1	2	5	2	58.10
2.660	27	1	2	3	33.67	1.5779	1	2	1	6	58.44
2.645	1	2	2	1	33.86	1.5775	2	0	6	1	58.44
2.634	6	0	1	4	34.01	1.5351	3	1	6	1	60.24
2.532	7	1	0	4	35.42	1.5266	1	1	5	4	60.61
2.440	7	2	2	2	36.80	1.5172	3	2	2	6	61.02
2.392	2	0	4	0	37.57	1.5066	1	4	2	2	61.50
2.378	4	2	1	3	37.79	1.5046	2	1	1	7	61.59
2.377	4	0	2	4	37.81	1.4837	3	3	4	3	62.55
2.337	11	0	4	1	38.49	1.4526	2	2	4	5	64.05
2.259	3	1	3	3	39.88	1.4517	1	1	2	7	64.09
2.204	3	1	4	1	40.91	1.4469	1	3	5	0	64.33
2.192	1	0	4	2	41.15	1.4271	1	1	6	3	65.33
2.136	5	0	1	5	42.27	1.4249	3	2	6	1	65.45
2.120	7	2	3	2	42.61	1.4211	1	4	3	2	65.65
2.112	12	2	0	4	42.77	1.4188	2	4	0	4	65.77
2.081	1	1	4	2	43.44	1.4082	1	3	0	6	66.32
2.078	4	0	3	4	43.51	1.4034	1	4	1	4	66.58
2.063	5	2	1	4	43.86	1.3966	2	3	4	4	66.94
2.005	4	3	1	2	45.18	1.3931	2	3	1	6	67.13
2.001	3	0	4	3	45.28	1.3747	1	1	3	7	68.15
1.9744	6	3	2	1	45.93	1.3502	1	4	2	4	68.99
1.9400	1	2	4	0	46.79	1.3525	2	4	4	1	69.44
1.9326	4	2	2	4	46.93	1.3493	1	1	6	4	69.62
1.9157	9	1	4	3	47.42	1.3298	1	2	4	6	70.80
1.9103	11	2	4	1	47.56	1.3100	1	4	1	5	72.03
1.8847	18	3	2	2	48.25	1.2963	1	4	3	4	72.92
1.8557	1	3	1	3	49.05	1.2957	1	1	5	6	72.95
1.8385	3	1	5	0	49.54	1.2894	2	0	6	5	73.37
1.8288	1	2	4	2	49.82	1.2850	1	1	4	7	73.66
1.8172	2	3	3	0	50.16	1.2844	1	3	6	1	73.70
1.8131	1	1	5	1	50.28	1.2769	1	4	4	3	74.20

Cesium Lithium Fluoride, $CsLiF_2$ (monoclinic)

Structure

Monoclinic, C2/c (15), Z=8 [Burns and Busing, 1965].

Lattice parameters

a=6.01±0.02, b=11.64±0.02, c=8.18±0.02Å, β=90°45′±5′ [ibid.]

Scattering factors

Li^{+1} [3.3.1A]; Cs°,F^{-1} [3.3.1A],corrected for real and imaginary dispersion [3.3.2B]

Thermal parameters

Isotropic: Cs 1.96; Li 2.50; F(1) 2.20; F(2) 2.40; F(3) 3.00.

Density

(calculated) 4.130 g/cm^3

Scale factor

10.28×10^4

Reference

Burns,J.H. and W.R. Busing (1965). Crystal structures of rubidium lithium fluoride, $RbLiF_2$, and cesium lithium fluoride, $CsLiF_2$, Inorg. Chem. 4, 1510-1512.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
5.82	28	0	2	0		15.22
4.74	42	0	2	1		18.70
4.49	47	-1	1	1		19.74
4.45	42	1	1	1		19.94
4.09	42	0	0	2		21.72
3.35	16	0	2	2		26.62
3.26	51	-1	1	2		27.30
3.23	51	1	1	2		27.60
3.04	91	-1	3	1		29.40
3.02	100	1	3	1		29.54
3.01	74	2	0	0		29.70
2.910	44	0	4	0		30.70
2.741	17	0	4	1		32.64
2.670	13	2	2	0		33.54
2.547	21	-2	2	1		35.20
2.529	29	2	2	1		35.46
2.469	86	0	2	3		36.36
2.436	25	-2	0	2	+	36.86
2.416	3	1	1	3		37.18
2.406	19	2	0	2		37.34
2.371	8	0	4	2		37.92
2.248	2	-2	2	2		40.08
2.223	1	2	2	2		40.54
2.100	7	-1	5	1	+	43.04
2.095	9	1	5	1		43.14
2.091	18	2	4	0		43.24
2.084	10	1	3	3		43.38
2.030	1	-2	4	1		44.60
2.021	2	2	4	1		44.82
1.9894	9	0	4	3		45.56
1.9403	7	0	6	0		46.78
1.9187	32	-2	2	3	+	47.34
1.9141	31	1	5	2	+	47.46
1.9020	15	1	1	4		47.78
1.8968	24	2	2	3		47.92
1.8682	8	-2	4	2		48.70
1.8546	6	2	4	2		49.08
1.7866	6	-3	1	2		51.08
1.7692	7	3	1	2		51.62
1.7527	7	0	6	2		52.14
1.7434	13	-3	3	1		52.44
1.7348	11	3	3	1		52.72
1.7008	1	-2	0	4		53.86
1.6800	2	2	0	4		54.58
1.6665	7	-2	4	3		55.06
1.6516	8	2	4	3		55.60
1.6300	11	2	6	0		56.40
1.5964	1	2	6	1		57.70
1.5809	2	0	6	3		58.32
1.5740	8	0	2	5	+	58.60

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.5715	8	1 7 1 +	58.70
1.5590	1	1 1 5	59.22
1.5177	2	-2 6 2	61.00
1.5105	2	2 6 2	61.32
1.5026	6	4 0 0	61.68
1.4917	9	-1 5 4	62.18
1.4904	9	1 7 2 +	62.24
1.4848	7	1 5 4	62.50
1.4663	3	-1 3 5	63.38
1.4581	3	1 3 5	63.78
1.4544	2	4 2 0 +	63.96
1.4324	2	0 8 1	65.06
1.4293	6	-3 1 4 +	65.22
1.4258	5	0 4 5	65.40
1.4189	4	3 5 2	65.76
1.4154	3	-4 0 2	65.94
1.4113	3	3 1 4	66.16
1.4075	2	0 6 4	66.36
1.4023	5	-2 2 5 +	66.64
1.3945	1	2 6 3	67.06
1.3875	4	2 2 5	67.44
1.3631	3	0 0 6	68.82
1.3350	3	4 4 0	70.48
1.3200	1	-4 4 1	71.40
1.3152	1	4 4 1	71.70
1.2941	1	-2 4 5	73.06
1.2904	4	-4 2 3	73.30
1.2835	2	0 8 3 +	73.76
1.2767	4	4 2 3	74.22
1.2734	3	-4 4 2	74.44
1.2656	2	-3 7 1	74.98
1.2627	3	-1 7 4 +	75.18
1.2593	3	1 7 4	75.42
1.2500	4	-1 9 1	76.08
1.2492	4	1 9 1	76.14
1.2472	3	-2 0 6	76.28
1.2347	2	0 4 6 +	77.20
1.2248	3	-3 5 4 +	77.94
1.2182	1	3 7 2	78.44
1.2133	2	3 5 4	78.82
1.2115	1	-3 3 5 +	78.96
1.2044	1	-4 4 3	79.52
1.1976	1	3 3 5	80.06
1.1936	1	4 4 3	80.38
1.1877	2	4 6 0	80.86
1.1831	2	-2 8 3	81.24
1.1779	2	2 8 3	81.68
1.1516	1	-5 1 2	83.96
1.1467	2	-2 4 6 +	84.40
1.1439	3	-4 6 2 +	84.66

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.82	25	0 2 0	15.21
4.74	40	0 2 1	18.70
4.50	45	-1 1 1	19.73
4.45	41	1 1 1	19.95
4.09	42	0 0 2	21.71
3.35	16	0 2 2	26.62
3.27	56	-1 1 2	27.29
3.23	55	1 1 2	27.60
3.04	92	-1 3 1	29.40
3.02	96	1 3 1	29.55
3.00	70	2 0 0	29.71
2.910	48	0 4 0	30.70
2.742	19	0 4 1	32.63
2.670	15	2 2 0	33.54
2.547	25	-2 2 1	35.21
2.529	32	2 2 1	35.46
2.469	100	0 2 3	36.36
2.440	1	-1 1 3	36.81
2.437	27	-2 0 2	36.86
2.417	1	1 1 3	37.17
2.406	22	2 0 2	37.34
2.371	9	0 4 2	37.92
2.248	2	-2 2 2	40.08
2.224	1	2 2 2	40.53
2.101	6	-1 5 1	43.02
2.099	2	-1 3 3	43.07
2.096	5	1 5 1	43.13
2.090	19	2 4 0	43.24
2.084	1	1 3 3	43.38
2.045	1	0 0 4	44.26
2.030	2	-2 4 1	44.61
2.021	2	2 4 1	44.81
1.9896	12	0 4 3	45.55
1.9400	9	0 6 0	46.79
1.9247	4	-3 1 1	47.18
1.9212	15	-1 5 2	47.27
1.9186	24	-2 2 3	47.34
1.9171	16	-1 1 4	47.38
1.9137	14	1 5 2	47.47
1.9134	4	3 1 1	47.48
1.9022	16	1 1 4	47.77
1.8966	24	2 2 3	47.93
1.8876	1	0 6 1	48.17
1.8682	10	-2 4 2	48.70
1.8545	8	2 4 2	49.08
1.7869	8	-3 1 2	51.07
1.7685	9	3 1 2	51.63
1.7528	9	0 6 2	52.14
1.7434	17	-3 3 1	52.44
1.7350	14	3 3 1	52.71

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7009	2	-2 0 4	53.86
1.6803	2	2 0 4	54.57
1.6662	11	-2 4 3	55.07
1.6516	11	2 4 3	55.60
1.6298	16	2 6 0	56.41
1.6006	1	-2 6 1	57.53
1.5962	1	2 6 1	57.71
1.5807	3	0 6 3	58.33
1.5748	7	0 2 5	58.57
1.5738	6	-1 7 1	58.61
1.5717	7	1 7 1	58.69
1.5692	1	-1 1 5	58.79
1.5590	1	1 1 5	59.22
1.5177	2	-2 6 2	61.00
1.5103	2	2 6 2	61.33
1.5024	9	4 0 0	61.69
1.4956	1	-3 5 1	62.00
1.4939	4	-1 7 2	62.08
1.4920	9	-1 5 4	62.17
1.4904	5	1 7 2	62.24
1.4903	1	3 5 1	62.25
1.4849	10	1 5 4	62.49
1.4662	4	-1 3 5	63.38
1.4579	4	1 3 5	63.79
1.4551	1	2 4 4	63.92
1.4547	1	4 2 0	63.95
1.4325	2	0 8 1	65.06
1.4295	5	-3 1 4	65.21
1.4291	2	4 2 1	65.23
1.4281	4	-3 5 2	65.28
1.4260	3	0 4 5	65.39
1.4189	5	3 5 2	65.76
1.4162	2	-4 0 2	65.90
1.4112	5	3 1 4	66.16
1.4074	1	0 6 4	66.37
1.4043	1	4 0 2	66.53
1.4033	1	-2 6 3	66.58
1.4021	7	-2 2 5	66.65
1.3946	1	2 6 3	67.06
1.3877	6	2 2 5	67.43
1.3761	1	-4 2 2	68.08
1.3632	5	0 0 6	68.81
1.3350	5	4 4 0	70.48
1.3273	1	0 2 6	70.95
1.3245	1	-1 1 6	71.12
1.3200	1	-4 4 1	71.40
1.3151	1	4 4 1	71.71
1.2940	1	-2 4 5	73.06
1.2902	7	-4 2 3	73.31
1.2836	3	0 8 3	73.75

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.2826	1	2 4 5	73.82
1.2767	7	4 2 3	74.22
1.2734	1	-4 4 2	74.44
1.2657	3	-3 7 1	74.97
1.2635	3	-1 7 4	75.13
1.2625	2	3 7 1	75.20
1.2592	3	1 7 4	75.42
1.2501	4	-1 9 1	76.08
1.2490	4	1 9 1	76.15
1.2476	2	-2 0 6	76.26
1.2354	2	2 0 6	77.15
1.2345	3	0 4 6	77.21
1.2249	4	-3 5 4	77.93
1.2240	2	-3 7 2	78.00
1.2199	1	-2 2 6	78.31
1.2182	2	3 7 2	78.44
1.2133	4	3 5 4	78.82
1.2115	1	-3 3 5	78.96
1.2084	1	2 2 6	79.20
1.2045	2	-4 4 3	79.51
1.1975	2	3 3 5	80.07
1.1935	2	4 4 3	80.39
1.1878	3	4 6 0	80.85
1.1831	4	-2 8 3	81.25
1.1778	4	2 8 3	81.69
1.1640	1	0 10 0	82.87
1.1569	1	-1 5 6	83.49
1.1516	1	-5 1 2	83.96
1.1468	1	-1 7 5	84.39
1.1466	1	-2 4 6	84.41
1.1442	1	-1 1 7	84.63
1.1439	2	-4 6 2	84.66
1.1435	2	5 1 2	84.69
1.1428	1	1 7 5	84.76
1.1389	3	-5 3 1	85.12
1.1387	1	1 1 7	85.13
1.1375	1	4 6 2	85.24
1.1371	1	2 4 6	85.28
1.1350	2	5 3 1	85.48
1.1195	1	0 10 2	86.95
1.1154	2	0 6 6	87.36
1.1024	3	-1 3 7	88.65
1.0975	3	1 3 7	89.15
1.0940	2	-4 2 5	89.52

Structure

Monoclinic, C2/c(15), Z=4 [Steinfink and Burns, 1964]

Lattice parameters

a=7.773±.005,b=7.540±.005,c=7.440±.005Å, β=124.25±0.1°[ibid.]

Scattering factors

F^{-1} [3.3.1A]; Cr^{+2}, Cr^{+3} [3.3.1B]

Thermal parameters

Isotropic:Cr^{+3} 0.49;Cr^{+2} 0.77;F^-(1) 1.41 F^-(2) 1.19; F^-(3) 1.64

Density

(calculated) 3.667 g/cm³

Scale factor

3.008 × 10^4

Reference

Steinfink,H. and J.H.Burns(1964).The crystal structure of Cr_2F_5, Acta Cryst. 17, 823-826.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
4.89	2	1	1	0		18.12
3.77	100	0	2	0		23.58
3.358	68	-2	0	2		26.52
3.321	5	-1	1	2		26.82
3.213	70	2	0	0		27.74
3.074	35	0	0	2		29.02
2.704	1	-2	2	1		33.10
2.507	14	-2	2	2		35.78
2.445	9	2	2	0		36.72
2.423	11	-3	1	2		37.08
2.383	3	0	2	2	+	37.72
2.354	4	-1	3	1		38.20
2.268	3	-1	1	3		39.70
2.211	4	1	1	2		40.78
2.146	2	-3	1	3		42.08
2.079	1	-1	3	2		43.50
2.060	4	3	1	0		43.92
1.9411	12	-4	0	2		46.76
1.8849	22	0	4	0		48.24
1.8504	18	-2	0	4		49.20
1.7925	2	-3	3	2		50.90
1.7769	14	2	0	2	+	51.38
1.7257	7	-4	2	2		53.02
1.7019	1	1	3	2		53.82
1.6961	1	-2	4	1		54.02

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
1.6789	4	-4	0	4		54.62
1.6609	13	-2	2	4		55.26
1.6434	12	-2	4	2		55.90
1.6258	11	2	4	0		56.56
1.6066	20	4	0	0	+	57.30
1.5373	5	0	0	4		60.14
1.5336	6	-4	2	4		60.30
1.5181	1	-5	1	3		60.98
1.4776	5	4	2	0		62.84
1.4235	3	0	2	4		65.52
1.3524	5	-4	4	2		69.44
1.3206	6	-2	4	4		71.36
1.3146	1	1	1	4		71.74
1.2931	6	2	4	2		73.12
1.2787	3	-6	0	4		74.08
1.2737	1	-1	5	3		74.42
1.2568	1	0	6	0		75.60
1.2537	3	-4	4	4	+	75.82
1.2349	1	-4	0	6		77.18
1.2227	4	4	4	0		78.10
1.2110	4	-6	2	4		79.00
1.1914	3	0	4	4		80.56
1.1897	2	-6	2	2	+	80.70
1.1769	2	-2	6	2	+	81.76
1.1736	3	-4	2	6		82.04
1.1703	2	2	6	0		82.32
1.1632	1	0	6	2		82.94
1.1563	1	2	0	4		83.54
1.1055	1	2	2	4		88.34
1.0728	1	-6	2	6		91.78
1.0708	1	6	0	0		92.00
1.0582	2	-6	4	4		93.42
1.0549	1	-4	6	2		93.80
1.0441	1	-6	4	2		95.08
1.0396	1	-2	6	4		95.62
1.0329	1	-4	4	6		96.44
1.0302	2	6	2	0		96.78
1.0261	1	2	6	2		97.30
1.0250	1	0	0	6		97.44
1.0060	1	-2	4	6	+	99.94
.9987	1	4	4	2		100.94
.9891	1	0	2	6	+	102.30
.9857	1	2	4	4		102.78
.9705	1	-8	0	4		105.06
.9399	1	-8	2	4		110.08
.9311	1	6	4	0		111.64
.9109	1	-8	2	6		115.48
.9074	1	-2	8	2		116.18
.9044	1	2	8	0		116.80
.9011	1	0	8	2		117.48
.9005	1	0	4	6		117.60

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
4.89	2	1	1	0	18.12
3.77	100	0	2	0	23.58
3.357	73	-2	0	2	26.53
3.322	4	-1	1	2	26.81
3.213	77	2	0	0	27.75
3.075	37	0	0	2	29.01
2.704	1	-2	2	1	33.10
2.507	16	-2	2	2	35.78
2.445	11	2	2	0	36.72
2.422	13	-3	1	2	37.09
2.383	3	0	2	2	37.72
2.380	2	-3	1	1	37.77
2.354	5	-1	3	1	38.20
2.269	4	-1	1	3	39.70
2.211	5	1	1	2	40.78
2.146	3	-3	1	3	42.07
2.079	1	-1	3	2	43.49
2.060	5	3	1	0	43.91
1.9973	1	2	2	1	45.37
1.9409	16	-4	0	2	46.76
1.8850	28	0	4	0	48.24
1.8504	23	-2	0	4	49.20
1.7927	3	-3	3	2	50.89
1.7772	17	2	0	2	51.37
1.7766	2	-3	1	4	51.39
1.7257	10	-4	2	2	53.02
1.7018	1	1	3	2	53.82
1.6956	1	-2	4	1	54.04
1.6787	5	-4	0	4	54.63
1.6611	18	-2	2	4	55.25
1.6437	17	-2	4	2	55.89
1.6301	1	3	3	0	56.40
1.6258	14	2	4	0	56.56
1.6075	8	2	2	2	57.26
1.6071	12	0	4	2	57.28
1.6063	13	4	0	0	57.31
1.5375	7	0	0	4	60.13
1.5336	5	-4	2	4	60.30
1.5182	1	-5	1	3	60.98
1.4777	8	4	2	0	62.83
1.4236	5	0	2	4	65.51
1.3522	8	-4	4	2	69.45
1.3205	3	-2	4	4	71.37
1.3144	1	1	1	4	71.75
1.2931	9	2	4	2	73.12
1.2789	4	-6	0	4	74.07
1.2736	1	-1	5	3	74.43
1.2567	2	0	6	0	75.61
1.2539	1	-6	0	2	75.80
1.2536	3	-4	4	4	75.82

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
1.2349	2	-4	0	6	77.18
1.2226	7	4	4	0	78.11
1.2111	6	-6	2	4	78.99
1.1914	5	0	4	4	80.56
1.1899	1	-6	2	2	80.69
1.1894	1	-2	0	6	80.73
1.1775	1	4	0	2	81.71
1.1769	2	-2	6	2	81.76
1.1735	4	-4	2	6	82.05
1.1703	1	2	6	0	82.32
1.1633	2	0	6	2	82.93
1.1564	2	2	0	4	83.54
1.1343	1	-2	2	6	85.55
1.1192	1	-6	0	6	86.99
1.1055	2	2	2	4	88.33
1.0729	2	-6	2	6	91.77
1.0708	2	6	0	0	92.00
1.0583	4	-6	4	4	93.41
1.0549	2	-4	6	2	93.81
1.0440	2	-6	4	2	95.09
1.0396	2	-2	6	4	95.62
1.0339	3	-4	4	6	96.44
1.0301	2	6	2	0	96.80
1.0261	2	2	6	2	97.30
1.0250	2	0	0	6	97.44
1.0060	1	-4	6	4	99.93
1.0059	1	-2	4	6	99.95
.9987	2	4	4	2	100.94
.9898	2	4	6	0	102.20
.9891	2	0	2	6	102.30
.9857	3	2	4	4	102.79
.9730	1	0	6	4	104.68
.9705	1	-8	0	4	105.07
.9623	1	-6	4	6	106.34
.9425	1	0	8	0	109.63
.9398	2	-8	2	4	110.09
.9311	3	6	4	0	111.64
.9252	1	-4	0	8	112.72
.9128	1	-8	0	2	115.11
.9109	2	-8	2	6	115.48
.9074	3	-2	8	2	116.18
.9044	2	2	8	0	116.80
.9011	3	0	8	2	117.48
.9005	3	0	4	6	117.61
.8985	3	-4	2	8	118.02
.8963	2	-6	6	4	118.49
.8886	2	4	0	4	120.19
.8883	2	-6	2	8	120.25
.8876	1	-6	6	2	120.41
.8871	2	-8	2	2	120.52

Structure

Orthorhombic, $P2_12_12_1$ (19), Z=4 [Gramaccioli and Marsh, 1966]

Lattice parameters

a=11.084, b=10.350, c=7.238Å [ibid.]

Scattering factors

H°, C°, N°, O° [3.3.1A]. Cu°[3.3.1A]corrected for the real part of the anomalous dispersion effect [3.3.2B]

Thermal parameters

Isotropic:Cu 1.71; C(1) 1.74; C(2) 1.70; C(3) 1.96; C(4) 2.19; C(5) 1.96; N 1.95; O(1) 2.18; O(2) 2.31; O(3) 2.09; O(4) 2.50; O(5) 2.71; O(6) 2.39; H(1) to H(11) inclusive, as given in Gramaccioli and Marsh [1966]

Density

(calculated) 1.957 g/cm³ [Gramaccioli and Marsh, 1966]

Scale factor

4.281×10^4

Reference

Gramaccioli,C.M. and R.E.Marsh (1966). The crystal structure of copper glutamate dihydrate, Acta Cryst. 21 594-600.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.56	72	1 1 0	11.70
5.93	17	0 1 1	14.92
5.54	52	2 0 0	15.98
5.23	100	1 1 1	16.94
5.18	23	0 2 0	17.12
4.89	38	2 1 0	18.14
4.69	2	1 2 0	18.92
4.40	1	2 0 1	20.16
4.21	42	0 2 1	21.08
4.05	63	2 1 1	21.94
3.93	63	1 2 1	22.58
3.78	3	2 2 0	23.50
3.62	6	0 0 2	24.58
3.440	18	1 0 2	25.88
3.351	3	2 2 1	26.58
3.290	12	3 0 1 +	27.08
3.264	12	1 1 2	27.30
3.136	11	3 1 1	28.44
3.114	5	0 3 1	28.64
3.029	1	2 0 2	29.46
3.006	15	3 2 0	29.70

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.998	26	1 3 1	29.78
2.966	7	3 2 2	30.10
2.928	4	2 3 0	30.50
2.908	1	2 1 2	30.72
2.864	14	1 2 2	31.20
2.771	4	4 0 0 +	32.28
2.715	1	2 3 1	32.96
2.676	4	4 1 0	33.46
2.615	2	2 2 2	34.26
2.586	11	3 0 2 +	34.66
2.509	7	3 1 2	35.76
2.497	5	0 3 2	35.94
2.443	1	4 2 0	36.76
2.436	3	0 4 1	36.86
2.379	12	1 4 1 +	37.78
2.349	7	0 1 3	38.28
2.313	18	3 2 2 +	38.90
2.299	8	1 1 3	39.16
2.276	12	2 3 2	39.56
2.231	6	2 4 1	40.40
2.212	2	2 0 3	40.76
2.186	1	0 2 3	41.26
2.163	9	2 1 3	41.72
2.152	3	4 1 2	41.94
2.146	8	1 2 3	42.08
2.120	3	5 0 1	42.62
2.105	1	0 4 2	42.94
2.077	9	5 1 1	43.54
2.070	7	3 3 2 +	43.70
2.069	7	1 4 2	43.72
2.034	9	1 5 0 +	44.50
2.025	3	4 2 2	44.72
1.9902	2	0 5 1	45.54
1.9828	2	3 1 3	45.72
1.9673	2	2 4 2	46.10
1.9593	1	1 5 1	46.30
1.8901	3	5 0 2	48.10
1.8820	2	3 2 3	48.32
1.8733	3	2 5 1	48.56
1.8596	9	5 1 2 +	48.94
1.8553	6	4 3 2	49.06
1.8476	1	6 0 0	49.28
1.8295	2	4 4 1	49.80
1.8192	7	4 0 3 +	50.10
1.8058	4	5 3 1 +	50.50
1.7971	4	0 5 2	50.76
1.7925	4	4 1 3	50.90
1.7737	5	1 5 2 +	51.48
1.7641	3	6 1 1	51.78
1.7597	2	1 1 4	51.92
1.7521	2	3 5 1	52.16

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7428	3	1 4 3 +	52.46
1.7251	1	0 6 0	53.04
1.7203	1	2 0 4	53.20
1.7167	1	4 2 3	53.32
1.7090	3	2 5 2 +	53.58
1.6967	1	2 1 4	54.00
1.6915	1	6 2 1	54.18
1.6880	2	1 2 4	54.30
1.6817	1	2 4 3	54.52
1.6760	2	4 4 2 +	54.72
1.6587	2	1 6 1	55.34
1.6472	2	2 6 0	55.76
1.6322	3	2 2 4	56.32
1.6164	1	4 5 1	56.92
1.6096	1	4 3 3	57.18
1.6055	1	3 1 4	57.34
1.5923	3	3 4 3	57.86
1.5883	4	6 3 1	58.02
1.5858	5	1 3 4	58.12
1.5681	2	6 2 2	58.84
1.5566	1	5 2 3	59.32
1.5504	1	3 2 4	59.58
1.5466	2	7 0 1	59.74
1.5424	2	1 6 2	59.92
1.5392	2	2 3 4	60.06
1.5276	1	3 6 1	60.56
1.5127	1	5 5 0	61.22
1.5079	1	4 5 2	61.44
1.4991	2	4 1 4 +	61.84
1.4818	2	7 2 1 +	62.64
1.4700	2	3 3 4	63.20
1.4646	1	4 6 0	63.46
1.4540	1	4 2 4	63.98
1.4364	3	1 7 1 +	64.86
1.4113	1	6 2 3	66.16
1.3960	1	5 5 2	66.98
1.3883	2	6 4 2 +	67.40
1.3761	1	3 4 4	68.08
1.3732	1	8 1 0	68.24
1.3575	1	4 6 2	69.14
1.3538	1	6 5 1	69.36
1.3521	2	2 2 5	69.46
1.3507	2	7 4 0	69.54
1.3490	2	8 1 1 +	69.64
1.3379	1	5 6 1	70.30
1.3366	1	3 1 5	70.38
1.3045	1	4 7 0	72.38
1.2820	1	5 5 3	73.86
1.2784	1	3 5 4	74.10
1.2607	1	0 7 3	75.32
1.2453	1	4 2 5	76.42

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.56	66	1 1 0	11.69
5.93	17	0 1 1	14.92
5.54	51	2 0 0	15.98
5.23	100	1 1 1	16.94
5.17	19	0 2 0	17.12
4.89	40	2 1 0	18.14
4.69	2	1 2 0	18.91
4.40	1	2 0 1	20.16
4.21	47	0 2 1	21.09
4.05	69	2 1 1	21.93
3.94	69	1 2 1	22.57
3.78	4	2 2 0	23.50
3.62	7	0 0 2	24.58
3.440	21	1 0 2	25.88
3.352	4	2 2 1	26.57
3.294	2	1 3 0	27.05
3.291	13	3 0 1	27.07
3.265	13	1 1 2	27.29
3.136	13	3 1 1	28.44
3.114	5	0 3 1	28.64
3.030	1	2 0 2	29.45
3.007	14	3 2 0	29.69
2.998	24	1 3 1	29.77
2.966	8	0 2 2	30.11
2.929	5	2 3 0	30.50
2.908	1	2 1 2	30.72
2.865	17	1 2 2	31.19
2.777	1	3 2 1	32.21
2.771	4	4 0 0	32.28
2.715	1	2 3 1	32.96
2.677	5	4 1 0	33.45
2.615	2	2 2 2	34.26
2.588	5	4 0 1	34.63
2.587	1	0 4 0	34.64
2.585	10	3 0 2	34.67
2.508	9	3 1 2	35.77
2.497	6	0 3 2	35.93
2.443	1	4 2 0	36.76
2.436	3	0 4 1	36.86
2.381	3	3 3 1	37.75
2.380	13	1 4 1	37.77
2.357	1	1 0 3	38.14
2.350	8	0 1 3	38.27
2.315	4	4 2 1	38.88
2.313	21	3 2 2	38.91
2.299	9	1 1 3	39.16
2.277	15	2 3 2	39.55
2.230	8	2 4 1	40.41
2.212	3	2 0 3	40.76
2.187	1	0 2 3	41.25

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.163	11	2 1 3	41.72
2.152	3	4 1 2	41.95
2.145	10	1 2 3	42.08
2.120	4	5 0 1	42.62
2.105	1	0 4 2	42.93
2.077	12	5 1 1	43.55
2.070	1	4 3 1	43.69
2.069	3	3 3 2	43.72
2.068	4	1 4 2	43.74
2.035	7	1 5 0	44.49
2.034	1	2 2 3	44.50
2.034	4	3 4 1	44.51
2.025	3	4 2 2	44.72
1.9902	3	0 5 1	45.54
1.9827	2	3 1 3	45.72
1.9677	2	2 4 2	46.09
1.9589	1	1 5 1	46.31
1.8903	4	5 0 2	48.09
1.8818	3	3 2 3	48.33
1.8731	4	2 5 1	48.56
1.8622	3	2 3 3	48.87
1.8596	11	5 1 2	48.94
1.8550	2	4 3 2	49.07
1.8473	1	6 0 0	49.29
1.8298	2	4 4 1	49.79
1.8196	5	4 0 3	50.09
1.8186	5	6 1 0	50.12
1.8060	3	5 3 1	50.49
1.8059	2	3 5 0	50.50
1.7968	5	0 5 2	50.77
1.7921	3	4 1 3	50.91
1.7756	1	5 2 2	51.42
1.7737	6	1 5 2	51.48
1.7636	4	6 1 1	51.79
1.7598	1	1 1 4	51.91
1.7522	3	3 5 1	52.16
1.7432	2	3 3 3	52.45
1.7426	3	1 4 3	52.47
1.7250	1	0 6 0	53.04
1.7201	1	2 0 4	53.21
1.7166	1	4 2 3	53.32
1.7092	4	2 5 2	53.57
1.7081	1	0 2 4	53.61
1.6969	1	2 1 4	53.99
1.6916	1	6 2 1	54.17
1.6882	2	1 2 4	54.29
1.6814	1	2 4 3	54.53
1.6780	1	0 6 1	54.65
1.6761	2	4 4 2	54.72
1.6591	2	1 6 1	55.33

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6471	3	2 6 0	55.77
1.6323	3	2 2 4	56.31
1.6165	2	4 5 1	56.92
1.6095	1	4 3 3	57.19
1.6054	1	3 1 4	57.35
1.5923	5	3 4 3	57.86
1.5888	2	6 3 1	58.00
1.5860	6	1 3 4	58.11
1.5680	2	6 2 2	58.84
1.5568	1	5 2 3	59.31
1.5504	2	3 2 4	59.58
1.5468	3	7 0 1	59.73
1.5420	2	1 6 2	59.94
1.5394	2	2 3 4	60.05
1.5278	1	3 6 1	60.55
1.5129	1	5 5 0	61.21
1.5076	1	4 5 2	61.45
1.4991	1	2 6 2	61.84
1.4991	2	4 1 4	61.84
1.4820	2	7 2 1	62.63
1.4809	1	5 5 1	62.68
1.4701	3	3 3 4	63.20
1.4644	1	4 6 0	63.47
1.4540	1	4 2 4	63.98
1.4457	1	3 5 3	64.39
1.4366	2	7 1 2	64.85
1.4364	3	1 7 1	64.86
1.4353	1	4 6 1	64.91
1.4349	1	3 6 2	64.93
1.4112	1	6 2 3	66.17
1.3959	1	5 5 2	66.98
1.3884	3	6 4 2	67.39
1.3872	2	4 3 4	67.46
1.3762	1	3 4 4	68.07
1.3732	2	8 1 0	68.24
1.3575	1	4 6 2	69.14
1.3540	1	6 5 1	69.35
1.3520	2	2 2 5	69.47
1.3506	1	7 4 0	69.55
1.3492	1	8 1 1	69.63
1.3487	1	3 7 1	69.66
1.3379	2	5 6 1	70.30
1.3365	1	3 1 5	70.38
1.3045	1	4 7 0	72.38
1.2818	1	5 5 3	73.88
1.2782	1	3 5 4	74.11
1.2607	1	0 7 3	75.32
1.2454	1	4 2 5	76.42
1.2421	1	6 6 1	76.65
1.2359	1	7 3 3	77.11

Structure

Monoclinic, C2/c (15),Z=4 [Robertson and Calvo, 1967]

Lattice parameters

a=6.876, b=8.113, c=9.162Å, β=109.54° [ibid.]

Polymorphism

The polymorph β-$Cu_2P_2O_7$ occurs at temperatures higher than about 66°C [ibid.]

Scattering factors

P°, O^{-1} [3.3.1A]
Cu^{+2} [3.3.1A] corrected for anomalous dispersion [3.3.2B]

Thermal parameters

Isotropic: Cu 0.94; P 0.75; O(1) 2.21; O(2) 1.29; O(3) 0.95; O(4) 1.36

Density

(calculated) 4.151 g/cm³

Scale factor

6.635×10^4

Reference

Robertson, B.E. and C. Calvo (1967). The crystal structure and phase transformation of α-$Cu_2P_2O_7$, Acta Cryst.22,665-72.

Note:

Using the structure data of Robertson and Calvo [1967], we were unable to duplicate their calculated structure factors, but the scaled integrated intensities agreed within 2%.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.06	6	1 1 0	17.50
4.97	6	-1 1 1	17.84
4.32	11	0 0 2	20.56
3.94	1	1 1 1	22.54
3.81	6	-1 1 2	23.30
3.67	2	0 2 1	24.22
3.241	2	2 0 0	27.50
3.144	100	-2 0 2	28.36
2.957	79	0 2 2	30.20
2.928	46	1 1 2	30.50
2.841	4	-1 1 3	31.46
2.621	2	-2 2 1	34.18
2.532	18	2 2 0	35.42
2.495	18	1 3 0	35.96
2.489	11	-1 3 1	36.06

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.293	2	-1 3 2	39.26
2.274	1	2 2 1	39.60
2.254	2	2 0 2	39.96
2.205	3	-1 1 4	40.90
2.175	7	-3 1 2	41.48
2.160	9	-2 0 4 +	41.78
2.087	7	3 1 0	43.32
2.049	17	1 3 2	44.16
2.030	3	-3 1 3 +	44.60
1.9706	7	2 2 2	46.02
1.9065	16	-2 2 4 +	47.66
1.8357	3	0 4 2	49.62
1.7478	6	-1 3 4	52.30
1.7330	8	-3 3 2	52.78
1.7043	1	-2 4 2	53.74
1.6874	6	3 3 0	54.32
1.6200	3	4 0 0	56.78
1.6107	2	-3 1 5	57.14
1.5814	4	-4 2 2	58.30
1.5725	7	-4 0 4 +	58.66
1.5701	9	2 0 4	58.76
1.5667	5	-4 2 1	58.90
1.5448	1	-4 2 3	59.82
1.5378	13	1 3 4 +	60.12
1.5190	3	-1 5 2	60.94
1.5168	2	-2 0 6	61.04
1.5043	2	4 2 0	61.60
1.4784	2	-2 4 4	62.80
1.4646	1	2 2 4	63.46
1.4487	5	3 3 2	64.24
1.4415	4	1 5 2	64.60
1.4383	3	0 0 6	64.76
1.4208	1	-2 2 6	65.66
1.3732	2	4 0 2	68.24
1.3551	2	-5 1 2 +	69.28
1.3521	4	0 6 0	69.46
1.3460	1	-5 1 3	69.82
1.3313	1	-5 1 1	70.70
1.3226	6	-1 3 6 +	71.24
1.3178	2	-3 5 2	71.54
1.3045	1	3 1 4	72.38
1.3008	1	4 2 2	72.62
1.2974	4	3 5 0 +	72.84
1.2895	1	-4 4 3	73.36
1.2539	1	-3 1 7	75.80
1.2523	2	-4 2 6	75.92
1.2423	4	-2 6 2 +	76.64
1.2258	1	-3 5 4	77.86
1.1887	1	-5 3 4	80.78
1.1687	1	5 3 0	82.46
1.1305	1	2 2 6	85.30

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.06	5	1 1 0	17.50
4.97	5	-1 1 1	17.83
4.32	10	0 0 2	20.56
3.94	1	1 1 1	22.54
3.81	6	-1 1 2	23.30
3.67	2	0 2 1	24.22
3.240	2	2 0 0	27.51
3.145	100	-2 0 2	28.35
2.956	62	0 2 2	30.21
2.929	44	1 1 2	30.50
2.841	4	-1 1 3	31.46
2.621	2	-2 2 1	34.18
2.532	20	2 2 0	35.43
2.496	19	1 3 0	35.95
2.484	1	-1 3 1	36.12
2.292	2	-1 3 2	39.27
2.274	1	2 2 1	39.60
2.255	2	2 0 2	39.96
2.204	3	-1 1 4	40.91
2.175	8	-3 1 2	41.49
2.161	9	-2 0 4	41.77
2.159	3	0 0 4	41.81
2.087	8	3 1 0	43.31
2.049	20	1 3 2	44.16
2.030	3	-3 1 3	44.60
2.028	1	0 4 0	44.64
1.9706	7	2 2 2	46.02
1.9069	18	-2 2 4	47.65
1.9056	2	0 2 4	47.68
1.8357	3	0 4 2	49.62
1.7478	6	-1 3 4	52.30
1.7329	10	-3 3 2	52.78
1.7045	2	-2 4 2	53.73
1.6877	8	3 3 0	54.31
1.6579	1	0 4 3	55.37
1.6200	3	4 0 0	56.78
1.6105	2	-3 1 5	57.15
1.5815	5	-4 2 2	58.29
1.5748	4	1 5 0	58.60
1.5726	6	-4 0 4	58.66
1.5703	7	2 0 4	58.75
1.5667	2	-4 2 1	58.90
1.5448	1	-4 2 3	59.82
1.5390	2	-3 3 4	60.07
1.5376	17	1 3 4	60.13
1.5190	4	-1 5 2	60.94
1.5168	1	-2 0 6	61.04
1.5045	2	4 2 0	61.59
1.4787	3	-2 4 4	62.79
1.4644	1	2 2 4	63.47

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.4487	7	3 3 2	64.24
1.4416	6	1 5 2	64.60
1.4391	1	0 0 6	64.72
1.4207	1	-2 2 6	65.66
1.3732	3	4 0 2	68.24
1.3633	1	-4 2 5	68.81
1.3562	1	0 2 6	69.21
1.3550	2	-5 1 2	69.29
1.3522	5	0 6 0	69.45
1.3460	1	-5 1 3	69.82
1.3313	1	-5 1 1	70.70
1.3240	3	-1 5 4	71.15
1.3226	8	-1 3 6	71.24
1.3175	2	-3 5 2	71.55
1.3045	1	3 1 4	72.38
1.3007	1	4 2 2	72.63
1.2979	2	1 1 6	72.81
1.2973	4	3 5 0	72.85
1.2895	2	-4 4 3	73.36
1.2798	1	5 1 0	74.01
1.2542	1	-3 1 7	75.78
1.2522	4	-4 2 6	75.92
1.2428	1	-4 4 4	76.60
1.2422	5	-2 6 2	76.64
1.2260	1	-3 5 4	77.85
1.2033	1	5 1 1	79.13
1.1888	2	-5 3 4	80.78
1.1772	1	2 0 6	81.74
1.1687	2	5 3 0	82.46
1.1305	2	2 2 6	85.90
1.1295	1	5 1 2	85.99
1.1168	1	-1 1 8	87.22
1.1043	1	-4 4 6	88.46
1.0988	1	-6 2 2	89.02
1.0861	1	4 2 4	90.34
1.0850	1	-5 1 7	90.45
1.0803	1	-4 0 8	90.97
1.0800	1	6 0 0	91.00
1.0793	1	0 0 8	91.07
1.0772	1	-3 5 6	91.30
1.0487	1	-5 5 2	94.53
1.0430	1	0 2 8	95.21
1.0411	2	-3 3 8	95.44
1.0253	1	-4 6 4	97.40
1.0248	2	3 5 4	97.47
1.0246	1	2 6 4	97.48
1.0215	2	1 5 6	97.88

Structure

Orthorhombic, Pbca (61), Z=8 [Williams, 1966]

Lattice parameters

a=10.857±0.002, b=24.447±0.005, c=8.756±0.002Å (published value,b=24.446±0.005Å) [ibid.]

Scattering factors

H°, O°, C° [Hanson et al., 1964]

Thermal parameters

Isotropic

C(1) 4.04; C(2) 5.17; C(3) 5.47; C(4) 5.56; C(5) 5.44; C(6) 4.75; C(7) 4.22; C(8) 5.18; C(9) 6.12; O(10) 6.06; O(11) 5.71; O(12) 4.87; O(13) 4.22; O(14) 4.15; O(15) 4.37; O(16) 5.71; O(17) 5.86; H(18) through H(29) as given by Williams [1966]

Density

(calculated) 1.281 g/cm^3 [Williams,1966]

Scale factor

13.32 × 10^4

Reference

Hanson, H.P., F. Herman, J.D. Lea, and S. Skillman (1964). HFS atomic scattering factors, Acta Cryst. 17, 1040-1044.

Williams, D.E. (1966). Crystal structure of dibenzoylmethane,Acta Cryst.21,340-9.

Note:

There has been a correction in this last reference. The x parameter for C(3) should be -0.07535.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
12.20	36	0 2 0	7.24
7.11	3	0 2 1	12.44
6.56	2	1 1 1	13.48
6.11	4	0 4 0	14.48
5.95	4	1 2 1	14.88
5.43	70	2 0 0	16.32
5.30	15	2 1 0	16.72
5.23	99	1 3 1	16.94
5.01	3	0 4 1	17.68
4.53	50	2 1 1	19.56
4.52	46	2 3 0	19.62
4.38	5	0 0 2	20.28
4.32	21	2 2 1	20.56
4.12	37	0 2 2	21.54
4.07	3	0 6 0	21.80
3.97	29	1 5 1	22.36
3.85	21	1 2 2	23.06
3.69	6	0 6 1	24.08
3.68	7	2 4 1	24.14
3.63	100	1 3 2	24.48
3.56	10	0 4 2	25.00
3.406	3	2 0 2	26.14
3.381	15	1 4 2	26.34
3.376	14	2 1 2	26.38
3.356	3	2 5 1	26.54
3.283	5	2 2 2	27.14
3.259	2	2 6 0	27.34
3.227	3	3 2 1	27.62
3.144	42	2 3 2	28.36
3.125	8	1 5 2	28.54
3.093	5	3 3 1	28.84
2.976	17	2 4 2 +	30.00
2.934	4	3 4 1	30.44
2.884	3	0 8 1	30.98
2.877	2	1 6 2	31.06
2.840	3	0 2 3	31.48
2.800	1	1 1 3	31.94
2.789	2	2 0 2	32.06
2.714	2	4 0 0	32.98
2.664	1	2 8 0	33.62
2.639	1	3 3 2	33.94
2.614	1	2 6 2	34.28
2.584	2	3 6 1	34.68
2.579	2	4 1 1	34.76
2.557	2	2 1 3 +	35.06
2.547	3	2 8 1	35.20
2.538	5	3 4 2 +	35.34
2.524	2	1 9 1	35.54
2.442	5	1 5 3 +	36.78
2.318	6	1 6 3	38.82

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.219	1	4 3 2	40.62
2.193	1	1 7 3	41.12
2.188	2	3 3 3	41.22
2.180	1	3 7 2	41.38
2.160	3	2 10 1	41.78
2.134	1	0 10 2	42.32
2.129	2	3 4 3	42.42
2.124	1	2 9 2	42.52
2.108	2	3 9 1	42.86
2.094	1	1 10 2	43.16
2.071	1	1 8 3	43.66
2.025	1	1 4 4	44.72
2.003	2	2 11 1	45.24
1.9844	2	0 12 1	45.68
1.9673	1	2 8 3	46.10
1.9286	1	0 6 4	47.08
1.9043	2	3 7 3	47.72
1.8923	1	5 3 2	48.04
1.8747	1	2 5 4	48.52
1.8233	1	3 8 3	49.98
1.8172	1	2 6 4	50.16
1.8125	1	1 13 1	50.30
1.8091	1	6 0 0	50.40
1.8051	1	6 1 0	50.52
1.7866	1	4 6 3	51.08
1.7788	1	4 10 1	51.32
1.7556	2	2 7 4	52.06
1.7490	2	3 5 4	52.26
1.7019	2	3 6 4	53.82

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
12.22	27	0 2 0	7.23
7.12	3	0 2 1	12.42
6.57	1	1 1 1	13.48
6.11	3	0 4 0	14.48
5.95	3	1 2 1	14.87
5.43	62	2 0 0	16.32
5.30	11	2 1 0	16.72
5.23	92	1 3 1	16.94
5.01	3	0 4 1	17.68
4.55	1	1 4 1	19.49
4.53	44	2 1 1	19.56
4.52	17	2 3 0	19.63
4.38	4	0 0 2	20.27
4.32	20	2 2 1	20.56
4.12	36	0 2 2	21.54
4.07	2	0 6 0	21.79
3.97	28	1 5 1	22.36
3.85	20	1 2 2	23.06
3.69	5	0 6 1	24.07
3.68	3	2 4 1	24.15
3.63	100	1 3 2	24.47
3.56	10	0 4 2	25.00
3.408	2	2 0 2	26.13
3.382	14	1 4 2	26.33
3.375	4	2 1 2	26.38
3.356	2	2 5 1	26.54
3.283	5	2 2 2	27.14
3.259	1	2 6 0	27.35
3.226	3	3 2 1	27.63
3.144	44	2 3 2	28.36
3.124	5	1 5 2	28.55
3.094	4	3 3 1	28.83
2.983	3	0 6 2	29.93
2.976	16	2 4 2	30.00
2.934	3	3 4 1	30.44
2.885	3	0 8 1	30.97
2.876	1	1 6 2	31.07
2.839	4	0 2 3	31.49
2.800	1	1 1 3	31.94
2.789	2	3 0 2	32.06
2.714	2	4 0 0	32.97
2.663	2	2 8 0	33.63
2.639	1	3 3 2	33.94
2.614	1	2 6 2	34.28
2.585	2	3 6 1	34.67
2.578	1	4 1 1	34.77
2.560	1	1 4 3	35.03
2.557	1	2 1 3	35.07
2.548	2	2 8 1	35.20
2.538	4	3 4 2	35.34

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.536	1	4 2 1	35.36
2.523	1	1 9 1	35.55
2.445	2	0 10 0	36.73
2.442	3	1 5 3	36.78
2.442	2	1 8 2	36.78
2.318	7	1 6 3	38.82
2.220	1	4 3 2	40.61
2.193	1	1 7 3	41.12
2.188	2	3 3 3	41.22
2.180	1	3 7 2	41.39
2.160	3	2 10 1	41.78
2.134	1	0 10 2	42.31
2.130	1	3 4 3	42.41
2.124	1	2 9 2	42.52
2.109	2	3 9 1	42.85
2.094	1	1 10 2	43.16
2.072	1	1 8 3	43.65
2.025	1	1 4 4	44.72
2.002	2	2 11 1	45.25
1.9842	2	0 12 1	45.68
1.9672	1	2 8 3	46.10
1.9283	1	0 6 4	47.09
1.9044	3	3 7 3	47.72
1.8921	1	5 3 2	48.05
1.8750	1	2 5 4	48.51
1.8232	1	3 8 3	49.98
1.8171	1	2 6 4	50.16
1.8128	1	1 13 1	50.29
1.8095	1	6 0 0	50.39
1.8046	1	6 1 0	50.54
1.7864	2	4 6 3	51.09
1.7786	1	4 10 1	51.33
1.7552	2	2 7 4	52.06
1.7491	2	3 5 4	52.26
1.7016	3	3 6 4	53.82

Structure

Monoclinic, Pn(7) or P2/n(13), Z=2 [Marezio et al., 1961].

Lattice parameters

a=9.651±0.001, b=6.525±0.001, c=7.923±0.001Å, β=93.65±0.02° [ibid.]

Scattering factors

Gd° [Thomas and Umeda, 1957], corrected for dispersion [Dauben and Templeton, 1955]
H°, O^{-1}, Cl^{-1} [3.3.1A]

Thermal parameters

Isotropic [Marezio et al., 1961]

Density

(calculated) 2.478 g/cm³ [Marezio et al., 1961]

Scale factor

$2.514 \times 10^{*}$

Additional patterns

1. P.D.F. card 3-0392 [Dow Chemical Co., Midland, Mich.]

Reference

Dauben, C.H. and D.H. Templeton (1955). A table of dispersion corrections for x-ray scattering of atoms, Acta Cryst. **8**, 841-842.

Marezio, M.,H.A. Plettinger, and W.H.Zachariasen (1961). The crystal structure of gadolinium trichloride hexahydrate, Acta Cryst. **14**, 234-236.

Thomas, L. H. and K. Umeda (1957). Atomic scattering factors calculated from the TFD atomic model,J.Chem.Phys.**26**,293-303.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.525	41	0 1 0	13.56
6.312	100	-1 0 1	14.02
5.925	100	1 0 1	14.94
5.401	71	1 1 0	16.40
5.029	66	0 1 1	17.62
4.813	49	2 0 0	18.42
4.535	36	-1 1 1	19.56
4.388	43	1 1 1	20.22
3.952	59	0 0 2	22.48
3.874	11	2 1 0	22.94

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.550	71	-2 1 1	25.06
3.411	63	2 1 1	26.10
3.381	16	0 1 2	26.34
3.262	3	0 2 0	27.32
3.252	2	-1 1 2	27.40
3.155	7	-2 0 2	28.26
3.138	7	1 1 2	28.42
3.089	27	1 2 0	28.88
3.044	4	-3 0 1	29.32
2.965	7	2 0 2	30.12
2.910	5	3 0 1	30.70
2.881	17	3 1 0	31.02
2.859	17	1 2 1	31.26
2.841	3	-2 1 2	31.46
2.758	5	-3 1 1	32.44
2.699	3	2 2 0 +	33.16
2.659	7	3 1 1	33.68
2.584	23	-2 2 1 +	34.68
2.528	18	2 2 1	35.48
2.517	11	0 2 2	35.64
2.502	10	1 0 3	35.86
2.460	16	-1 2 2	36.50
2.444	2	0 1 3	36.74
2.407	22	1 2 2 +	37.32
2.403	31	-1 1 3	37.40
2.395	25	-3 1 2	37.52
2.336	20	1 1 3	38.50
2.288	40	3 2 0	39.34
2.267	11	3 1 2	39.72
2.260	9	4 1 0	39.86
2.233	23	-2 1 3	40.36
2.207	13	-4 1 1	40.86
2.194	4	2 2 2	41.10
2.175	5	0 3 0 +	41.48
2.139	5	4 1 1	42.22
2.129	20	2 1 3	42.42
2.123	12	1 3 0	42.54
2.118	11	-4 0 2	42.66
2.104	3	-3 0 3	42.96
2.098	3	0 3 1	43.08
2.056	16	-1 3 1	44.00
2.051	12	0 2 3	44.12
2.042	12	1 3 1	44.32
2.021	10	-3 2 2	44.82
2.001	4	4 0 2 +	45.28
1.9820	3	2 3 0 +	45.74
1.9771	9	0 0 4 +	45.86
1.9427	17	3 2 2	46.72
1.9372	11	-2 3 1 +	46.86
1.9209	7	-2 2 3	47.28
1.9156	5	4 1 2	47.42
1.9058	13	0 3 2 +	47.68

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.8998	11	-5 0 1	47.84
1.8916	7	0 1 4 +	48.06
1.8784	2	-1 1 4	48.42
1.8711	3	-2 0 4	48.62
1.8596	4	4 2 1	48.94
1.8539	6	2 2 3	49.10
1.8483	4	5 1 0	49.26
1.8448	3	5 0 1	49.36
1.8357	1	1 1 4	49.62
1.8240	7	-5 1 1	49.96
1.7984	1	-2 1 4	50.72
1.7892	4	2 0 4 +	51.00
1.7756	4	5 1 1 +	51.42
1.7685	6	-4 1 3 +	51.64
1.7534	1	2 3 2	52.12
1.7422	3	3 3 1	52.48
1.6903	1	0 2 4	54.22
1.6806	6	-1 2 4	54.56
1.6755	6	-3 1 4 +	54.74
1.6665	5	4 1 3	55.06
1.6643	6	-1 3 3	55.14
1.6593	4	5 2 0	55.32
1.6499	4	1 2 4	55.66
1.6413	6	1 3 3 +	55.98
1.6311	2	0 4 0	56.36
1.6138	2	4 3 0	57.02
1.6050	7	6 0 0 +	57.36
1.5883	4	3 1 4 +	58.02
1.5779	4	-4 0 4 +	58.44
1.5735	3	1 4 1	58.62
1.5585	3	-5 1 3 +	59.24
1.5476	2	-6 1 1	59.70
1.5448	3	2 4 0	59.82

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.525	39	0 1 0	13.56
6.312	97	-1 0 1	14.02
5.929	100	1 0 1	14.93
5.402	72	1 1 0	16.40
5.033	70	0 1 1	17.61
4.816	53	2 0 0	18.41
4.537	38	-1 1 1	19.55
4.388	46	1 1 1	20.22
3.953	68	0 0 2	22.47
3.875	12	2 1 0	22.93
3.552	86	-2 1 1	25.05
3.411	73	2 1 1	26.10
3.381	16	0 1 2	26.34
3.263	3	0 2 0	27.31
3.246	1	-1 1 2	27.45
3.156	7	-2 0 2	28.26
3.137	8	1 1 2	28.42
3.090	34	1 2 0	28.87
3.043	4	-3 0 1	29.33
2.965	8	2 0 2	30.12
2.911	6	3 0 1	30.69
2.881	20	3 1 0	31.02
2.858	21	1 2 1	31.27
2.841	3	-2 1 2	31.46
2.758	6	-3 1 1	32.44
2.701	2	2 2 0	33.14
2.699	2	2 1 2	33.16
2.658	10	3 1 1	33.69
2.584	5	-1 0 3	34.68
2.584	24	-2 2 1	34.68
2.529	23	2 2 1	35.47
2.516	12	0 2 2	35.65
2.502	11	1 0 3	35.86
2.459	22	-1 2 2	36.51
2.444	2	0 1 3	36.75
2.411	15	1 2 2	37.27
2.408	14	4 0 0	37.31
2.403	25	-1 1 3	37.40
2.394	25	-3 1 2	37.54
2.336	27	1 1 3	38.50
2.288	52	3 2 0	39.34
2.267	12	3 1 2	39.72
2.259	9	4 1 0	39.87
2.233	30	-2 1 3	40.36
2.207	18	-4 1 1	40.85
2.194	5	2 2 2	41.11
2.175	6	0 3 0	41.48
2.172	1	3 2 1	41.54
2.139	6	4 1 1	42.22
2.129	25	2 1 3	42.42

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.122	2	1 3 0	42.58
2.117	13	-4 0 2	42.67
2.104	3	-3 0 3	42.95
2.097	2	0 3 1	43.10
2.056	22	-1 3 1	44.00
2.050	5	0 2 3	44.14
2.042	15	1 3 1	44.32
2.021	13	-3 2 2	44.82
2.002	2	-3 1 3	45.25
2.001	5	4 0 2	45.29
1.9854	2	1 2 3	45.66
1.9822	2	2 3 0	45.73
1.9767	10	0 0 4	45.87
1.9763	3	3 0 3	45.88
1.9426	24	3 2 2	46.72
1.9373	1	4 2 0	46.86
1.9347	6	-2 3 1	46.92
1.9210	10	-2 2 3	47.28
1.9128	1	4 1 2	47.49
1.9056	16	0 3 2	47.68
1.9044	3	-4 2 1	47.72
1.8996	7	-5 0 1	47.85
1.8918	6	0 1 4	48.05
1.8915	3	3 1 3	48.06
1.8781	3	-1 1 4	48.43
1.8710	4	-2 0 4	48.62
1.8598	5	4 2 1	48.93
1.8536	7	2 2 3	49.11
1.8475	1	5 1 0	49.28
1.8447	4	5 0 1	49.36
1.8353	1	1 1 4	49.63
1.8238	10	-5 1 1	49.96
1.7985	1	-2 1 4	50.72
1.7909	3	-2 3 2	50.95
1.7891	4	2 0 4	51.00
1.7760	2	-4 2 2	51.41
1.7751	4	5 1 1	51.43
1.7695	3	-3 3 1	51.61
1.7681	6	-4 1 3	51.65
1.7536	1	2 3 2	52.11
1.7423	5	3 3 1	52.48
1.6906	1	0 2 4	54.21
1.6808	9	-1 2 4	54.55
1.6775	1	0 3 3	54.67
1.6751	6	-3 1 4	54.75
1.6667	6	4 1 3	55.05
1.6641	7	-1 3 3	55.15
1.6587	4	5 2 0	55.34
1.6499	5	1 2 4	55.66
1.6416	2	-5 2 1	55.97

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6415	7	1 3 3	55.97
1.6312	3	0 4 0	56.35
1.6140	2	4 3 0	57.01
1.6083	1	1 4 0	57.23
1.6058	3	5 2 1	57.33
1.6052	5	6 0 0	57.35
1.6046	3	-5 0 3	57.38
1.6045	1	-2 3 3	57.38
1.6006	1	-4 2 3	57.53
1.5881	7	3 1 4	58.03
1.5793	2	-1 4 1	58.38
1.5779	5	-4 0 4	58.44
1.5766	1	-1 0 5	58.49
1.5728	2	1 4 1	58.65
1.5604	2	-5 2 2	59.16
1.5588	2	6 1 0	59.23
1.5582	3	-5 1 3	59.25
1.5476	2	-6 1 1	59.70
1.5450	2	2 4 0	59.81

Structure
Monoclinic, $P2_1/a$ (14), Z=2 [Brown,1966]

Lattice parameters
a=8.489, b=15.581, c=5.598Å, β=102.9°
(published value: b=15.580Å) [ibid.]

Scattering factors
H^0, C^0, N^0, O^0 [3.3.1A]

Thermal parameters
Anisotropic for carbon,nitrogen, and oxygen,isotropic for hydrogen [Brown,1966]

Density
(calculated) 1.207 g/cm³

Scale factor
1.235×10^4

Reference
Brown, C.J. (1966). Further refinement of the crystal structure of hexamethylenediammonium adipate,Acta Cryst.21,185-190

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.78	37	0 2 0	11.36
7.31	11	1 1 0	12.10
5.67	2	1 2 0	15.62
5.45	1	0 0 1	16.24
4.85	8	1 1 -1	18.26
4.40	17	1 3 0	20.18
4.27	93	1 2 -1	20.78
4.01	99	1 1 1	22.16
4.00	96	2 1 0	22.20
3.72	2	2 0 -1	23.90
3.65	72	2 2 0	24.34
3.64	100	1 3 -1	24.42
3.52	10	1 4 0	25.26
3.358	3	2 2 -1	26.52
3.236	20	2 3 0 +	27.54
3.097	2	1 4 -1	28.80
2.992	1	2 0 1	29.84
2.938	6	2 1 1	30.40

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.915	1	1 5 0	30.64
2.738	1	1 1 -2	32.68
2.728	4	0 0 2	32.80
2.720	2	3 1 0	32.90
2.706	3	0 5 1	33.08
2.687	7	0 1 2 +	33.32
2.660	14	1 5 -1	33.66
2.596	7	0 6 0 +	34.52
2.566	2	3 2 -1	34.94
2.555	2	2 0 -2	35.10
2.521	5	2 1 -2	35.58
2.489	9	2 5 0 +	36.06
2.482	5	1 6 0	36.16
2.428	2	2 2 -2	37.00
2.405	1	1 1 2	37.36
2.389	1	2 5 -1	37.62
2.324	1	1 2 2	38.72
2.314	2	1 6 -1	38.88
2.293	9	2 3 -2	39.26
2.264	1	1 4 -2	39.78
2.242	2	3 1 1	40.18
2.229	9	3 4 -1	40.44
2.199	1	2 6 0	41.00
2.129	2	2 6 -1	42.42
2.064	3	1 4 2 +	43.82
2.060	3	0 7 1	43.92
2.056	3	2 1 2	44.00
2.051	4	4 1 0 +	44.12
2.005	2	2 2 2 +	45.18
1.9754	1	2 5 -2	45.90
1.9593	2	3 4 1 +	46.30
1.8476	3	4 1 -2	49.28
1.8329	1	3 5 1	49.70
1.8267	3	4 4 0	49.88
1.8064	2	0 1 3 +	50.48
1.7628	3	1 8 1	51.82
1.7251	1	2 8 -1	53.04
1.7215	1	3 7 -1	53.16
1.7072	2	3 6 1	53.64
1.6829	1	1 4 -3	54.48
1.6637	1	3 2 -3	55.16
1.6380	1	4 4 1 +	56.10
1.6009	1	1 5 -3	57.52

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.79	34	0 2 0	11.35
7.31	10	1 1 0	12.10
5.67	2	1 2 0	15.61
5.46	1	0 0 1	16.23
4.86	8	1 1 -1	18.26
4.40	18	1 3 0	20.17
4.27	100	1 2 -1	20.77
4.01	98	1 1 1	22.15
4.00	41	2 1 0	22.21
3.72	2	2 0 -1	23.89
3.65	67	2 2 0	24.34
3.64	80	1 3 -1	24.42
3.52	12	1 4 0	25.25
3.358	4	2 2 -1	26.53
3.242	4	1 3 1	27.49
3.236	21	2 3 0	27.54
3.098	3	1 4 -1	28.80
2.931	1	2 0 1	29.85
2.937	7	2 1 1	30.41
2.916	1	1 5 0	30.63
2.739	1	1 1 -2	32.67
2.728	4	0 0 2	32.80
2.716	1	3 1 0	32.95
2.706	3	0 5 1	33.08
2.691	1	2 4 -1	33.27
2.687	8	0 1 2	33.31
2.650	17	1 5 -1	33.66
2.600	3	3 2 0	34.47
2.597	7	0 6 0	34.51
2.566	2	3 2 -1	34.93
2.555	2	2 0 -2	35.09
2.521	6	2 1 -2	35.58
2.492	1	1 5 1	36.01
2.489	11	2 5 0	36.05
2.478	2	1 6 0	36.23
2.428	2	2 2 -2	37.00
2.405	1	1 1 2	37.35
2.389	1	2 5 -1	37.62
2.324	1	1 2 2	38.72
2.315	2	1 6 -1	38.87

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.292	12	2 3 -2	39.27
2.264	1	1 4 -2	39.78
2.243	2	3 1 1	40.17
2.229	12	3 4 -1	40.43
2.199	1	2 6 0	41.00
2.179	1	3 1 -2	41.40
2.149	1	1 7 0	42.00
2.129	2	2 6 -1	42.41
2.065	2	3 5 0	43.80
2.064	2	1 4 2	43.82
2.061	2	0 7 1	43.90
2.057	3	2 1 2	43.99
2.053	2	0 5 2	44.08
2.051	2	4 1 0	44.13
2.048	2	3 5 -1	44.18
2.041	1	1 7 -1	44.36
2.026	2	3 3 -2	44.68
2.005	2	2 2 2	45.19
1.9757	1	2 5 -2	45.89
1.9614	1	1 7 1	46.25
1.9589	1	3 4 1	46.31
1.9434	1	4 3 -1	46.70
1.9101	1	2 7 -1	47.57
1.8957	1	1 8 0	47.95
1.8473	5	4 1 -2	49.29
1.8328	1	3 5 1	49.70
1.8270	3	4 4 0	49.87
1.8065	2	0 1 3	50.47
1.8054	1	4 0 1	50.51
1.7630	4	1 8 1	51.81
1.7255	2	2 8 -1	53.03
1.7220	1	3 7 -1	53.14
1.7075	3	3 6 1	53.63
1.6828	1	1 4 -3	54.48
1.6639	1	3 2 -3	55.15
1.6396	1	1 9 -1	56.04
1.6380	1	4 4 1	56.10
1.6009	2	1 5 -3	57.52

Structure
Monoclinic, $P2_1/c$ (14), Z=4 [Lundberg, 1966]

Lattice parameters
a=7.956, b=11.856, c=12.078 Å, β=113°58′
±.005 ±.005 ±.005 ±2′
[ibid.]

Scattering factors
Zn^0 [Thomas,and Umeda, 1957], corrected for the real part of the dispersion correction, [Dauben and Templeton,1955].
N^0, C^0, Cl^- [Berghuis et al.,1955]

Thermal parameters
Isotropic [Lundberg, 1966]

Density
(calculated)
1.73 g/cm³ [Lundberg,1966]

Scale factor
7.339×10^4

Reference

Berghuis,J.,IJ.M.Haanappel,M.Potters, B.O. Loopstra,C.H.MacGillavry,and A.L.Veenendaal (1955). New calculations of atomic scattering factors,Acta Cryst.8,478-483.

Dauben,C.H.and D.H.Templeton (1955). A table of dispersion corrections for x-ray scattering of atoms,Acta Cryst.8,841-842

Lundberg,B.K.S.(1966). The crystal structure of Di-imidazole-zinc(II) Dichloride Acta Cryst. 21, 901-909.

Thomas, L. H. and K. Umeda (1957). Atomic scattering factors calculated from the TFD atomic model, J.Chem. Phys. 26, 293-303.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
7.261	2	1	0	0		12.18
6.440	13	-1	1	1		13.74
6.197	100	1	1	0		14.28
5.925	5	0	2	0		14.94
5.514	11	0	0	2		16.06
5.224	48	0	2	1		16.96
5.087	92	-1	1	2		17.42
4.746	2	1	1	1		18.68
4.691	1	-1	2	1		18.90
4.081	2	-1	2	2		21.76
4.037	21	0	2	2		22.00
3.900	12	1	2	1		22.78
3.792	2	-1	1	3		23.44
3.760	10	-2	1	1		23.64
3.720	50	0	3	1	+	23.90
3.648	15	-2	1	2		24.38
3.636	28	2	0	0		24.46
3.553	29	1	1	2		25.04
3.512	16	-1	3	1	+	25.34
3.474	7	2	1	0		25.62
3.316	17	-1	2	3		26.86
3.220	15	-2	2	2	+	27.68
3.142	1	1	3	1		28.38
3.125	5	0	2	3		28.54
2.998	1	2	1	1		29.78
2.965	16	0	4	0		30.12
2.925	2	-1	1	4		30.54
2.863	8	0	4	1		31.22
2.817	4	-2	0	4		31.74
2.800	1	-2	3	1		31.94
2.769	3	1	1	3		32.30
2.759	4	0	0	4		32.42
2.753	5	-2	3	2		32.50
2.744	4	1	4	0		32.60
2.741	5	-2	1	4		32.64
2.693	4	0	3	3		33.24
2.676	2	2	3	0		33.46
2.650	3	-3	0	2		33.80
2.611	1	0	4	2		34.32
2.586	11	-3	1	2	+	34.66
2.545	2	-2	2	4		35.24
2.531	4	2	1	2		35.44
2.501	2	0	2	4		35.88
2.399	2	-1	3	4		37.46
2.379	4	-3	2	1	+	37.78
2.374	8	3	1	0	+	37.86
2.319	4	1	4	2		38.80
2.311	12	-3	1	4	+	38.94
2.294	2	-2	3	4		39.24
2.290	2	1	0	4		39.32

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.265	3	-1 5 1	39.76
2.254	2	1 5 0	39.96
2.248	4	1 1 4	40.08
2.221	3	-2 4 3 +	40.58
2.192	3	-2 2 5	41.14
2.186	4	-1 5 2	41.26
2.170	2	0 1 5 +	41.58
2.156	2	1 5 1	41.86
2.146	3	-3 3 3	42.06
2.142	3	2 4 1	42.16
2.052	2	-1 3 5	44.10
2.047	3	2 2 3	44.22
2.040	4	-1 5 3	44.36
2.017	1	-2 5 2	44.90
2.001	3	1 5 2 +	45.28
1.9919	1	-3 2 5	45.50
1.9820	2	-4 0 2	45.74
1.9763	4	0 6 0 +	45.88
1.9209	1	3 1 2	47.28
1.9171	3	-4 0 4 +	47.38
1.8827	1	1 1 5	48.30
1.8798	2	-4 2 2	48.38
1.8646	3	-3 3 5	48.80
1.8603	3	0 6 2	48.92
1.8553	3	-3 1 6	49.06
1.8462	2	-2 4 5	49.32
1.8413	2	2 1 4	49.46
1.8288	2	-4 2 1	49.82
1.8233	2	1 5 3	49.98
1.8172	4	4 0 0	50.16
1.8131	3	-2 5 4	50.28
1.7775	1	2 2 4	51.36
1.7679	4	-2 6 1 +	51.66
1.7565	2	2 4 3 +	52.02
1.7490	2	2 5 2 +	52.26
1.7379	2	-3 5 3 +	52.62
1.7306	1	-4 2 5	52.86
1.7179	4	1 3 5	53.28
1.7025	1	-2 6 3	53.80
1.6715	2	-3 5 4 +	54.88
1.6665	2	2 6 1	55.06
1.6560	1	-2 2 7	55.44
1.6505	3	-3 1 7	55.64
1.6467	3	-4 4 2 +	55.78
1.6221	1	-1 7 2	56.70
1.6174	2	1 1 6 +	56.88
1.6081	1	3 5 1	57.24
1.5710	1	2 6 2	58.72
1.5585	1	-5 1 2 +	59.24
1.5495	1	4 4 0	59.62

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.270	2	1 0 0	12.16
6.439	13	-1 1 1	13.74
6.198	100	1 1 0	14.28
5.928	5	0 2 0	14.93
5.518	11	0 0 2	16.05
5.222	51	0 2 1	16.96
5.088	97	-1 1 2	17.41
4.747	2	1 1 1	18.68
4.690	1	-1 2 1	18.91
4.084	2	-1 2 2	21.74
4.039	25	0 2 2	21.99
3.901	13	1 2 1	22.78
3.792	2	-1 1 3	23.44
3.759	11	-2 1 1	23.65
3.726	18	1 0 2	23.86
3.721	44	0 3 1	23.90
3.648	12	-2 1 2	24.38
3.635	29	2 0 0	24.47
3.555	35	1 1 2	25.03
3.514	8	0 1 3	25.33
3.513	11	-1 3 1	25.33
3.475	7	2 1 0	25.61
3.317	20	-1 2 3	26.86
3.295	1	-2 2 1	27.04
3.229	1	-2 1 3	27.60
3.220	18	-2 2 2	27.68
3.142	1	1 3 1	28.38
3.126	6	0 2 3	28.53
2.998	1	2 1 1	29.78
2.964	20	0 4 0	30.13
2.925	2	-1 1 4	30.54
2.863	10	0 4 1	31.22
2.817	5	-2 0 4	31.74
2.799	1	-2 3 1	31.95
2.770	4	1 1 3	32.29
2.759	3	0 0 4	32.42
2.752	4	-2 3 2	32.51
2.745	1	1 4 0	32.60
2.741	4	-2 1 4	32.65
2.693	5	0 3 3	33.24
2.675	2	2 3 0	33.47
2.650	3	-3 0 2	33.79
2.611	1	0 4 2	34.31
2.590	2	2 0 2	34.60
2.586	14	-3 1 2	34.65
2.544	2	-2 2 4	35.25
2.531	5	2 1 2	35.44
2.501	3	0 2 4	35.87
2.399	3	-1 3 4	37.46
2.382	2	-1 4 3	37.74

Calculated Pattern *(Integrated)*						
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
2.380	3	-3	2	1	37.77
2.374	5	3	1	0	37.86
2.374	2	2	2	2	37.87
2.320	4	1	4	2	38.79
2.311	7	1	3	3	38.94
2.311	8	-3	1	4	38.94
2.308	3	0	4	3	38.99
2.294	1	-2	3	4	39.24
2.289	2	1	0	4	39.32
2.265	3	-1	5	1	39.76
2.254	2	1	5	0	39.96
2.248	5	1	1	4	40.08
2.225	2	-1	2	5	40.51
2.221	3	-2	4	3	40.58
2.192	4	-2	2	5	41.15
2.186	4	-1	5	2	41.27
2.171	1	-3	3	1	41.56
2.170	2	0	1	5	41.58
2.156	2	1	5	1	41.86
2.146	3	-3	3	3	42.06
2.142	3	2	4	1	42.15
2.069	1	0	2	5	43.72
2.052	2	-1	3	5	44.10
2.046	3	2	2	3	44.22
2.040	4	-1	5	3	44.37
2.017	1	-2	5	2	44.91
2.001	1	-2	0	6	45.28
2.001	3	1	5	2	45.29
1.9917	1	-3	2	5	45.50
1.9820	2	-4	0	2	45.74
1.9760	3	0	6	0	45.89
1.9757	2	-3	4	2	45.89
1.9209	1	3	1	2	47.28
1.9172	3	-4	0	4	47.38
1.9142	1	3	3	1	47.46
1.8834	1	1	1	5	48.28
1.8797	2	-4	2	2	48.38
1.8645	3	-3	3	5	48.80
1.8603	2	0	6	2	48.92
1.8548	3	-3	1	6	49.08
1.8459	3	-2	4	5	49.33
1.8406	1	2	1	4	49.48

Calculated Pattern *(Integrated)*						
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
1.8291	2	-4	2	1	49.81
1.8226	1	1	5	3	50.00
1.8175	4	4	0	0	50.15
1.8140	1	-2	5	4	50.25
1.7887	1	-4	1	5	51.02
1.7775	1	2	2	4	51.36
1.7718	1	-1	6	3	51.54
1.7703	2	0	4	5	51.58
1.7685	3	-2	6	1	51.64
1.7671	2	-3	5	2	51.68
1.7565	1	-2	6	2	52.02
1.7564	1	2	4	3	52.02
1.7515	1	-3	5	1	52.18
1.7490	2	2	5	2	52.26
1.7384	1	-3	5	3	52.60
1.7376	1	4	2	0	52.63
1.7306	2	-4	2	5	52.86
1.7179	6	1	3	5	53.28
1.7027	2	-2	6	3	53.79
1.6870	1	-1	5	5	54.34
1.6741	1	0	7	1	54.79
1.6714	2	-3	5	4	54.89
1.6661	1	2	6	1	55.08
1.6560	2	-2	2	7	55.44
1.6506	2	-3	1	7	55.64
1.6476	1	-4	4	2	55.75
1.6470	1	1	5	4	55.77
1.6464	1	-4	4	3	55.79
1.6451	1	-4	3	5	55.84
1.6220	1	-1	7	2	56.71
1.6177	1	-2	6	4	56.87
1.6172	1	1	1	6	56.89
1.6080	1	3	5	1	57.24
1.5711	1	2	6	2	58.72
1.5605	1	2	2	5	59.16
1.5585	2	-5	1	2	59.24
1.5494	1	4	4	0	59.62
1.5444	1	-4	4	5	59.84
1.5358	2	-3	3	7	60.20
1.5237	1	0	2	7	60.74
1.4770	1	-1	7	4	62.87

Structure
Hexagonal, $R\bar{3}$ (148), Z=18 [Burns and Gordon, 1966]

Lattice parameters
a=13.29±0.01, c=8.91±0.01Å [ibid.]

Scattering factors
Li^+, Be^{+2}, F^- [3.3.1A]

Thermal parameters
Anisotropic [Burns and Gordon, 1966]

Density
(calculated) 2.169 g/cm^3

Scale factor
9.496 × 10^4

Additional patterns
1. PDF card 6-0557 [Thilo and Lehmann, 1949]

Reference

Burns, J.H. and E.K.Gordon (1966). Refinement of the crystal structure of Li_2BeF_4 Acta Cryst. 20, 135-138.

Thilo, E. and H.-A. Lehmann (1949). Über das System LiF-BeF_2 und seine Beziehungen zum System MgO-SiO_2, Z. Anorg. Chem., 258, 332-355.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
6.64	38	1 1 0	13.32
4.15	9	0 1 2	21.38
3.91	23	2 1 1 +	22.74
3.84	20	3 0 0	23.16
3.52	2	2 0 2	25.26
3.321	56	2 2 0	26.82
3.112	4	1 2 2 +	28.66
3.006	1	3 1 -1	29.70
2.738	2	4 0 1	32.68
2.712	31	1 1 -3 +	33.00
2.512	23	4 1 0 +	35.72
2.348	100	0 3 3 +	38.30
2.272	1	3 2 -2	39.64
2.215	95	3 3 0 +	40.70
2.187	3	1 0 4	41.24
2.045	2	5 0 2	44.26
1.9545	2	4 2 2	46.42
1.9179	15	1 4 -3 +	47.36
1.8427	8	2 5 0 +	49.42
1.8267	1	3 1 -4	49.88
1.7756	2	3 3 3 +	51.42
1.7416	2	4 3 -2 +	52.50
1.7221	1	6 1 -1	53.14
1.7025	2	2 0 5 +	53.80
1.6489	2	1 2 5 +	55.70
1.6112	15	6 0 3 +	57.12
1.5710	2	6 2 1	58.72
1.5561	4	2 4 4 +	59.34
1.5245	5	1 7 0 +	60.70
1.5150	2	1 5 -4 +	61.12
1.5026	1	2 6 2	61.68
1.4848	7	0 0 6	62.50
1.4540	2	4 5 -1 +	63.98
1.3562	14	7 1 -3 +	69.22
1.3500	2	5 1 -5	69.58
1.3030	6	3 6 3 +	72.48
1.2787	4	9 0 0	74.08
1.2333	4	3 3 6 +	77.30
1.2130	3	5 5 -3 +	78.84

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.64	34	1 1 0	13.31
4.15	10	0 1 2	21.37
3.91	15	2 1 1	22.73
3.91	11	1 2 -1	22.73
3.84	21	3 0 0	23.16
3.52	2	2 0 2	25.26
3.322	64	2 2 0	26.81
3.112	2	1 2 2	28.66
3.112	2	2 1 -2	28.66
3.005	1	3 1 -1	29.70
2.738	1	4 0 1	32.68
2.711	18	1 1 3	33.01
2.711	19	1 1 -3	33.01
2.512	17	4 1 0	35.72
2.512	11	1 4 0	35.72
2.349	58	3 0 3	38.29
2.349	67	0 3 3	38.29
2.271	1	3 2 -2	39.65
2.229	1	0 5 1	40.44
2.215	100	3 3 0	40.70
2.214	11	2 2 3	40.71
2.214	9	2 2 -3	40.71
2.187	2	1 0 4	41.25
2.045	3	5 0 2	44.25
1.9546	3	4 2 2	46.42
1.9178	9	1 4 3	47.36
1.9178	9	1 4 -3	47.36
1.8430	8	5 2 0	49.41
1.8430	4	2 5 0	49.41
1.8267	1	3 1 -4	49.88
1.7756	2	3 3 3	51.42
1.7756	1	3 3 -3	51.42
1.7614	1	4 0 4	51.87
1.7416	1	3 4 2	52.50
1.7416	2	4 3 -2	52.50
1.7221	2	6 1 -1	53.14

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7026	1	2 3 -4	53.80
1.7023	2	2 0 5	53.81
1.6490	1	1 2 5	55.69
1.6490	1	2 1 -5	55.69
1.6114	12	6 0 3	57.11
1.6114	10	0 6 3	57.11
1.5711	3	6 2 1	58.72
1.5562	3	2 4 4	59.34
1.5562	1	4 2 -4	59.34
1.5560	1	1 3 -5	59.35
1.5560	2	3 1 5	59.35
1.5245	5	1 7 0	60.70
1.5245	3	7 1 0	60.70
1.5152	1	1 5 -4	61.11
1.5150	1	0 4 5	61.12
1.5026	1	2 6 2	61.68
1.4850	11	0 0 6	62.49
1.4539	2	4 5 -1	63.98
1.4539	1	5 4 1	63.98
1.3562	3	1 7 -3	69.22
1.3562	7	7 1 3	69.22
1.3562	3	1 7 3	69.22
1.3562	8	7 1 -3	69.22
1.3557	2	2 2 6	69.24
1.3557	2	2 2 -6	69.24
1.3497	1	5 1 -5	69.60
1.3030	1	6 3 3	72.48
1.3030	4	3 6 3	72.48
1.3030	3	3 6 -3	72.48
1.3030	2	6 3 -3	72.48
1.2788	6	9 0 0	74.07
1.2558	1	2 8 0	75.67
1.2334	4	3 3 6	77.29
1.2334	4	3 3 -6	77.29
1.2131	3	5 5 -3	78.84
1.2131	3	5 5 3	78.84

Structure
Monoclinic, C2/c (15), Z=8 [Burns and Busing, 1965]

Lattice parameters
a=5.83±0.01, b=11.16±0.02, c=7.86±0.02Å, β=94°55′ [ibid.]

Scattering factors
Li^{+1} [3.3.1A]; Rb°,F^{-1} [3.3.1A], corrected for real and imaginary dispersion, [3.3.2B]

Thermal parameters
Isotropic: Rb 1.73; Li 2.50; F(1) 1.40; F(2) 1.80; F(3) 2.10

Density
(calculated) 3.40 g/cm³

Scale factor
4.815×10^4

Reference
Burns,J.H. and W.R. Busing (1965). Crystal structures of rubidium lithium fluoride, $RbLiF_2$, and cesium lithium fluoride, $CsLiF_2$, Inorg. Chem. 4, 1510-1512.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
5.58	29	0	2	0		15.88
5.15	6	1	1	0		17.20
4.54	31	0	2	1		19.52
4.46	39	-1	1	1		19.88
4.16	22	1	1	1		21.34
3.91	32	0	0	2		22.70
3.24	50	-1	1	2		27.52
3.20	18	0	2	2		27.82
3.01	36	1	1	2		29.66
2.955	55	-1	3	1		30.22
2.904	63	2	0	0		30.76
2.863	90	1	3	1		31.22
2.789	52	0	4	0		32.06
2.629	16	0	4	1		34.08
2.576	13	2	2	0		34.80
2.505	15	-2	2	1		35.82
2.435	45	-2	0	2		36.88
2.394	51	2	2	1		37.54
2.365	100	0	2	3		38.02
2.272	7	0	4	2		39.64
2.261	3	1	1	3		39.84
2.242	12	2	0	2		40.18
2.232	3	-2	2	2		40.38
2.083	3	1	5	0	+	43.40
2.053	5	-1	3	3		44.08
2.029	9	-1	5	1		44.62
2.012	15	2	4	0		45.02
1.9985	7	1	5	1		45.34
1.9217	4	2	4	1		47.26
1.9073	23	-2	2	3	+	47.64
1.8908	2	-3	1	1		48.08
1.8784	10	-1	1	4		48.42
1.8632	14	-1	5	2		48.84
1.8596	12	0	6	0		48.94
1.8343	13	-2	4	2		49.66
1.8165	6	1	5	2	+	50.18
1.8111	3	0	6	1		50.34
1.7853	9	1	1	4		51.12
1.7749	4	-3	1	2		51.44
1.7679	15	2	2	3		51.66
1.7478	4	2	4	2		52.30
1.7049	15	-3	3	1		53.72
1.6920	1	-2	0	4		54.16
1.6800	6	0	6	2		54.58
1.6604	6	3	1	2		55.28
1.6516	5	3	3	1		55.60
1.6413	8	-2	4	3		55.98
1.5662	8	2	6	0		58.92
1.5623	8	2	0	4		59.08
1.5495	6	2	4	3		59.62

Calculated Pattern *(Peak heights)*						
d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
1.5222	1	2	6	1		60.80
1.5150	4	-1	7	1	+	61.12
1.5079	4	0	2	5		61.44
1.5021	6	1	7	1		61.70
1.4878	1	-3	3	3		62.36
1.4780	3	-2	6	2		62.82
1.4548	3	-3	5	1		63.94
1.4520	7	4	0	0		64.08
1.4487	7	-1	5	4		64.24
1.4423	3	-1	7	2		64.56
1.4316	2	2	6	2		65.10
1.4277	6	-3	1	4	+	65.30
1.4200	5	1	7	2	+	65.70
1.4052	7	1	5	4		66.48
1.4015	6	-4	0	2		66.68
1.3857	7	-2	2	5		67.54
1.3757	1	1	3	5		68.10
1.3715	1	-2	6	3	+	68.34
1.3655	2	0	4	5		68.66
1.3634	4	4	2	1	+	68.80
1.3599	2	-4	2	2		69.00
1.3419	4	3	5	2		70.06
1.3383	3	-1	7	3		70.28
1.3121	2	3	1	4		71.90
1.3051	3	0	0	6		72.34
1.2953	3	2	2	5		72.98
1.2883	3	4	4	0	+	73.44
1.2826	4	-4	2	3		73.82
1.2732	1	-2	4	5		74.46
1.2559	1	4	4	1		75.66
1.2523	2	-4	4	2		75.92
1.2341	1	2	8	1		77.24
1.2304	4	0	8	3	+	77.52
1.2261	3	-3	7	1		77.84
1.2229	3	-1	7	4		78.08
1.2100	3	-3	5	4		79.08
1.2016	4	-1	3	1		79.74
1.1966	5	4	2	3	+	80.14
1.1934	3	-3	7	2		80.40
1.1822	2	0	4	6		81.32
1.1561	2	3	7	2		83.56
1.1541	2	2	0	6		83.74
1.1496	1	-2	8	3		84.14
1.1445	1	4	6	0		84.60
1.1369	1	3	5	4		85.30
1.1259	1	-2	4	6		86.34
1.1217	2	-1	5	6	+	86.74
1.1190	2	-4	6	2		87.00
1.1161	3	2	8	3	+	87.28
1.1107	2	-5	3	1	+	87.82
1.0920	1	-4	2	5		89.72

Calculated Pattern *(Integrated)*					2θ(°) λ = 1.54056 Å
d (Å)	*I*	*hkl*			
5.58	22	0	2	0	15.87
5.15	4	1	1	0	17.20
4.54	24	0	2	1	19.52
4.46	31	-1	1	1	19.88
4.16	18	1	1	1	21.33
3.92	28	0	0	2	22.69
3.24	44	-1	1	2	27.52
3.21	16	0	2	2	27.81
3.01	32	1	1	2	29.66
2.956	53	-1	3	1	30.21
2.904	56	2	0	0	30.76
2.863	64	1	3	1	31.21
2.790	49	0	4	0	32.05
2.628	15	0	4	1	34.09
2.576	13	2	2	0	34.79
2.504	15	-2	2	1	35.83
2.435	46	-2	0	2	36.89
2.403	1	-1	1	3	37.39
2.394	49	2	2	1	37.54
2.364	100	0	2	3	38.03
2.272	7	0	4	2	39.63
2.260	2	1	1	3	39.85
2.242	12	2	0	2	40.18
2.231	2	-2	2	2	40.39
2.083	3	1	5	0	43.40
2.081	1	2	2	2	43.46
2.053	5	-1	3	3	44.08
2.029	9	-1	5	1	44.62
2.012	16	2	4	0	45.02
1.9982	7	1	5	1	45.35
1.9214	4	2	4	1	47.27
1.9075	18	-2	2	3	47.63
1.9061	10	0	4	3	47.67
1.8906	2	-3	1	1	48.09
1.8781	11	-1	1	4	48.43
1.8632	14	-1	5	2	48.84
1.8600	7	0	6	0	48.93
1.8344	14	-2	4	2	49.66
1.8185	3	3	1	1	50.12
1.8163	5	1	5	2	50.19
1.8097	1	0	6	1	50.38
1.7856	11	1	1	4	51.11
1.7750	3	-3	1	2	51.44
1.7676	17	2	2	3	51.67
1.7479	4	2	4	2	52.30
1.7049	18	-3	3	1	53.72
1.6925	1	-2	0	4	54.16
1.6801	6	0	6	2	54.58
1.6606	7	3	1	2	55.27
1.6515	5	3	3	1	55.60

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.6414	9	-2 4 3	55.93
1.5663	9	2 6 0	58.92
1.5625	4	2 0 4	59.07
1.5497	7	2 4 3	59.61
1.5224	2	2 6 1	60.79
1.5151	2	-1 7 1	61.11
1.5148	2	0 6 3	61.13
1.5079	5	0 2 5	61.44
1.5022	6	1 7 1	61.70
1.4876	1	-3 3 3	62.37
1.4780	4	-2 6 2	62.82
1.4548	3	-3 5 1	63.94
1.4521	8	4 0 0	64.07
1.4491	5	-1 5 4	64.22
1.4422	3	-1 7 2	64.56
1.4316	1	2 6 2	65.10
1.4279	5	-3 1 4	65.29
1.4275	3	-1 3 5	65.31
1.4212	1	3 5 1	65.64
1.4201	6	1 7 2	65.69
1.4053	8	1 5 4	66.48
1.4012	3	-4 0 2	66.69
1.3859	10	-2 2 5	67.53
1.3757	2	1 3 5	68.10
1.3734	1	0 8 1	68.23
1.3713	1	-2 6 3	68.35
1.3657	2	0 4 5	68.67
1.3637	3	4 2 1	68.78
1.3633	2	2 4 4	68.81
1.3590	1	-4 2 2	69.05
1.3419	5	3 5 2	70.06
1.3381	1	-1 7 3	70.29
1.3120	2	3 1 4	71.90
1.3052	4	0 0 6	72.34
1.2953	3	2 2 5	72.98
1.2888	1	-1 1 6	73.41
1.2881	3	4 4 0	73.45
1.2826	5	-4 2 3	73.82
1.2731	1	-2 4 5	74.46
1.2558	2	4 4 1	75.67
1.2522	2	-4 4 2	75.93
1.2344	1	2 8 1	77.22
1.2306	1	-2 0 6	77.50
1.2303	3	0 8 3	77.52
1.2261	3	-3 7 1	77.84
1.2227	3	-1 7 4	78.10
1.2099	4	-3 5 4	79.09
1.2016	5	-1 9 1	79.74
1.1967	5	4 2 3	80.13
1.1960	2	1 7 4	80.18

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.1952	3	1 9 1	80.26
1.1928	1	-3 7 2	80.44
1.1916	1	-4 4 3	80.54
1.1822	3	0 4 6	81.32
1.1562	2	3 7 2	83.55
1.1541	1	2 0 6	83.74
1.1497	2	-2 8 3	84.13
1.1446	2	4 6 0	84.59
1.1369	2	3 5 4	85.30
1.1259	1	-2 4 6	86.33
1.1218	1	4 4 3	86.73
1.1217	1	-1 5 6	86.74
1.1132	2	-4 6 2	86.98
1.1168	2	2 8 3	87.22
1.1160	1	0 10 0	87.29
1.1158	2	3 3 5	87.31
1.1106	2	-5 3 1	87.82
1.1098	1	-1 7 5	87.90
1.0929	2	-4 2 5	89.72

Structure
Tetragonal, $I4_1/a$ (88), Z=16 [Brunton, 1966]

Lattice parameters
a=14.885±0.002, c=6.547±0.001Å
(published value: a=14.884Å) [ibid.]

Scattering factors
Li^{+1}, and F^{-1} [3.3.1A]
U^{+4} [Cromer and Waber, 1965], corrected for dispersion using $\Delta f'=-4$ and $\Delta f''=16$

Thermal parameters
Anisotropic for uranium, isotropic for fluorine and lithium [Brunton, 1966]

Density
(calculated) 6.23 g/cm^3 [ibid.]

Scale factor
205.3×10^4

Additional patterns

1. PDF card 10-121 [Insley et al., 1956]. This card represents data for $Li_7U_6F_{31}$ which is very close in composition.

Reference

Brunton, G. (1966). The crystal structure of $LiUF_5$, Acta Cryst. 21, 814-817.

Cromer, D.T. and J.T. Waber (1965). Scattering factors computed from relativistic Dirac-Slater wave functions, Acta Cryst. 18, 104-109.

Insley, H., T.N. McVay, R.E. Thoma and G. D. White (1956). Optical properties and x-ray diffraction data for some inorganic fluoride and chloride compounds, ORNL-2192, pg.30, Oak Ridge National Laboratory, Tennessee.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
7.44	1	0	2	0		11.88
5.99	24	0	1	1		14.78
5.26	88	2	2	0		16.84
4.67	100	2	1	1	+	19.00
3.96	50	0	3	1		22.46
3.493	49	2	3	1	+	25.48
3.329	64	4	2	0	+	26.76
3.162	46	1	4	1	+	28.20
2.996	52	0	2	2		29.80
2.779	18	2	2	2		32.18
2.711	20	0	5	1	+	33.02
2.546	11	5	2	1	+	35.22
2.481	1	0	6	0		36.18
2.354	8	6	2	0	+	38.20
2.334	2	4	2	2		38.54
2.292	9	1	6	1	+	39.28
2.179	1	5	1	2		41.40
2.102	16	3	6	1	+	43.00
2.073	10	2	1	3	+	43.62
2.064	29	6	4	0	+	43.82
2.051	47	4	4	2		44.12
2.022	2	0	7	1		44.78
1.9977	10	0	3	3		45.36
1.9771	13	0	6	2		45.86
1.9513	11	7	2	1		46.50
1.9294	8	2	3	3	+	47.06
1.9110	18	6	2	2	+	47.54
1.8675	15	4	1	3	+	48.72
1.8610	20	0	8	0		48.90
1.8302	7	6	5	1	+	49.78
1.7769	11	4	7	1	+	51.38
1.7603	11	0	5	3	+	51.90
1.7553	7	6	6	0		52.06
1.7125	5	5	2	3	+	53.46
1.6834	8	8	3	1	+	54.46
1.6370	4	0	0	4		56.14
1.6290	4	1	6	3	+	56.44
1.5809	13	2	8	2	+	58.32
1.5676	7	6	7	1	+	58.86
1.5633	7	2	2	4		59.04
1.5561	3	3	6	3		59.34
1.5462	6	6	6	2		59.76
1.5341	6	5	8	1	+	60.28
1.5231	1	9	7	3		60.76
1.4921	4	7	2	3		62.16
1.4835	1	8	4	2		62.56
1.4725	6	4	9	1	+	63.08
1.4688	11	4	2	4	+	63.26
1.4597	5	10	2	0	+	63.70
1.4447	2	10	1	1	+	64.44

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.4356	2	6 5 3 +	64.90
1.4094	3	4 7 3 +	66.26
1.3930	2	10 3 1	67.14
1.3821	3	4 10 0 +	67.74
1.3693	1	7 8 1 +	68.46
1.3617	4	8 3 3 +	68.90
1.3551	10	0 10 2 +	69.28
1.3466	2	6 9 1 +	69.78
1.3436	4	2 6 4 +	69.96
1.3330	2	10 2 2 +	70.60
1.3252	1	0 11 1	71.08
1.3155	3	8 8 0	71.68
1.3045	3	2 11 1 +	72.38
1.2980	3	6 7 3 +	72.80
1.2847	2	2 1 5	73.68
1.2826	6	6 4 4 +	73.82
1.2787	5	8 5 3 +	74.08
1.2764	3	10 6 0 +	74.24
1.2732	2	4 10 2	74.46
1.2662	1	0 3 5	74.94
1.2484	3	2 3 5 +	76.20
1.2426	3	4 9 3 +	76.62
1.2309	4	1 4 5 +	77.48
1.2290	6	0 8 4	77.62
1.2256	4	10 1 3	77.88
1.2235	3	12 2 0 +	78.04
1.2146	2	12 1 1 +	78.72
1.1986	3	7 10 1 +	79.98
1.1959	2	6 6 4	80.20
1.1936	2	10 3 3	80.38
1.1892	2	6 10 2 +	80.74
1.1834	2	5 2 5 +	81.22
1.1786	1	7 8 3	81.62
1.1689	1	11 6 1	82.44
1.1641	1	9 6 3 +	82.86
1.1545	1	1 6 5	83.70
1.1365	2	2 11 3 +	85.34
1.1276	2	3 6 5 +	86.16
1.1151	2	2 13 1 +	87.38
1.1095	3	6 12 0 +	87.94
1.1075	7	4 12 2 +	88.14
1.1027	1	7 2 5	88.62
1.0988	2	11 4 3 +	89.02
1.0953	5	10 8 2 +	89.38
1.0909	1	10 9 1 +	89.84
1.0893	3	2 10 4 +	90.00
1.0794	3	0 2 6 +	91.06
1.0757	2	1 12 3 +	91.46
1.0681	2	2 2 6 +	92.30
1.0646	1	7 10 3	92.70

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
7.44	1	0 2 0	11.88
5.99	27	0 1 1	14.77
5.26	100	2 2 0	16.83
4.67	91	2 1 1	19.00
4.67	25	1 2 1	19.00
3.95	63	0 3 1	22.47
3.492	3	3 2 1	25.49
3.492	62	2 3 1	25.49
3.328	46	4 2 0	26.76
3.328	37	2 4 0	26.76
3.161	31	4 1 1	28.20
3.161	31	1 4 1	28.20
2.996	71	0 2 2	29.79
2.780	25	2 2 2	32.18
2.710	3	4 3 1	33.03
2.710	3	3 4 1	33.03
2.710	23	0 5 1	33.03
2.546	11	5 2 1	35.21
2.546	4	2 5 1	35.21
2.481	2	0 6 0	36.18
2.354	7	6 2 0	38.21
2.354	6	2 6 0	38.21
2.334	3	4 2 2	38.54
2.292	3	6 1 1	39.27
2.292	11	1 6 1	39.27
2.179	2	5 1 2	41.41
2.102	1	6 3 1	43.00
2.102	23	3 6 1	43.00
2.074	1	1 2 3	43.61
2.074	13	2 1 3	43.61
2.064	22	6 4 0	43.82
2.064	21	4 6 0	43.82
2.051	70	4 4 2	44.12
2.022	2	0 7 1	44.78
1.9976	15	0 3 3	45.36
1.9772	19	0 6 2	45.86
1.9516	17	7 2 1	46.49
1.9293	1	3 2 3	47.06
1.9293	11	2 3 3	47.06
1.9109	15	6 2 2	47.54
1.9109	13	2 6 2	47.54
1.8676	12	4 1 3	48.72
1.8676	10	1 4 3	48.72
1.8505	29	0 8 0	48.91
1.8299	10	6 5 1	49.79
1.8299	1	5 6 1	49.79
1.7769	1	8 1 1	51.38
1.7769	7	7 4 1	51.38
1.7769	8	4 7 1	51.38
1.7769	2	1 8 1	51.38

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.7601	3	4 3 3	51.91
1.7601	4	3 4 3	51.91
1.7601	13	0 5 3	51.91
1.7542	1	6 6 0	52.09
1.7128	5	5 2 3	53.45
1.7128	3	2 5 3	53.45
1.6836	7	8 3 1	54.46
1.6836	6	3 8 1	54.46
1.6367	7	0 0 4	56.15
1.6287	2	6 1 3	56.45
1.6287	5	1 6 3	56.45
1.5807	8	8 2 2	58.33
1.5807	16	2 8 2	58.33
1.5675	3	9 2 1	58.86
1.5675	6	6 7 1	58.86
1.5675	2	2 9 1	58.86
1.5629	6	2 2 4	59.06
1.5559	5	3 6 3	59.35
1.5462	10	6 6 2	59.76
1.5339	5	8 5 1	60.29
1.5339	6	5 8 1	60.29
1.5230	1	0 7 3	60.76
1.4921	6	7 2 3	62.16
1.4835	1	8 4 2	62.56
1.4726	4	9 4 1	63.08
1.4726	5	4 9 1	63.08
1.4688	6	2 4 4	63.26
1.4688	9	4 2 4	63.26
1.4596	5	10 2 0	63.71
1.4596	4	2 10 0	63.71
1.4446	4	10 1 1	64.45
1.4446	1	1 10 1	64.45
1.4356	2	6 5 3	64.90
1.4356	2	5 6 3	64.90
1.4095	3	7 4 3	66.25
1.4095	3	4 7 3	66.25
1.3931	4	10 3 1	67.14
1.3820	2	10 4 0	67.75
1.3820	3	4 10 0	67.75
1.3693	1	8 7 1	68.46
1.3693	1	7 8 1	68.46
1.3615	3	8 3 3	68.91
1.3615	3	3 8 3	68.91
1.3550	7	8 6 2	69.29
1.3550	4	6 8 2	69.29
1.3550	10	0 10 2	69.29
1.3467	1	9 6 1	69.78
1.3467	2	6 9 1	69.78
1.3438	3	6 2 4	69.95
1.3438	4	2 6 4	69.95

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.3331	2	10 2 2	70.59
1.3331	1	2 10 2	70.59
1.3252	2	0 11 1	71.08
1.3157	7	8 8 0	71.67
1.3046	1	10 5 1	72.37
1.3046	2	5 10 1	72.37
1.3046	4	2 11 1	72.37
1.2979	1	9 2 3	72.81
1.2979	3	6 7 3	72.81
1.2979	2	2 9 3	72.81
1.2848	2	2 1 5	73.67
1.2825	7	6 4 4	73.83
1.2825	4	4 6 4	73.83
1.2786	4	8 5 3	74.09
1.2786	3	5 8 3	74.09
1.2764	2	10 6 0	74.24
1.2764	1	6 10 0	74.24
1.2732	1	4 10 2	74.46
1.2660	2	0 3 5	74.95
1.2484	1	11 4 1	76.20
1.2484	1	4 11 1	76.20
1.2481	3	2 3 5	76.22
1.2425	3	9 4 3	76.63
1.2425	3	4 9 3	76.63
1.2309	3	4 1 5	77.48
1.2309	3	1 4 5	77.48
1.2289	11	0 8 4	77.63
1.2255	3	10 1 3	77.88
1.2235	3	12 2 0	78.03
1.2235	1	2 12 0	78.03
1.2147	3	12 1 1	78.71
1.2147	2	1 12 1	78.71
1.1988	3	7 10 1	79.96
1.1986	2	0 5 5	79.98
1.1967	1	6 6 4	80.13
1.1936	2	10 3 3	80.38
1.1892	1	10 6 2	80.74
1.1892	3	6 10 2	80.74
1.1835	1	12 3 1	81.21
1.1833	1	2 5 5	81.22
1.1833	2	5 2 5	81.22
1.1785	1	7 8 3	81.63
1.1689	3	11 6 1	82.45
1.1640	1	9 6 3	82.87
1.1640	1	6 9 3	82.87
1.1546	1	1 6 5	83.70
1.1500	1	0 11 3	84.10
1.1365	1	10 5 3	85.33
1.1365	1	5 10 3	85.33
1.1365	2	2 11 3	85.33

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.1279	2	0 13 1	86.15
1.1277	2	3 6 5	86.17
1.1151	1	2 13 1	87.38
1.1150	1	0 7 5	87.40
1.1095	2	12 6 0	87.94
1.1095	3	6 12 0	87.94
1.1074	8	12 4 2	88.15
1.1074	8	4 12 2	88.15
1.1027	2	7 2 5	88.62
1.0988	1	11 4 3	89.02
1.0988	1	4 11 3	89.02
1.0953	7	10 8 2	89.38
1.0953	4	8 10 2	89.38
1.0909	1	10 9 1	89.83
1.0909	1	9 10 1	89.83
1.0894	2	10 2 4	90.00
1.0894	3	2 10 4	90.00
1.0796	3	0 2 6	91.04
1.0794	1	11 8 1	91.06
1.0794	1	8 11 1	91.06
1.0792	2	6 5 5	91.08
1.0756	1	12 1 3	91.48
1.0756	2	1 12 3	91.48
1.0684	2	2 2 6	92.26
1.0681	1	4 7 5	92.31
1.0681	1	7 4 5	92.31
1.0645	3	7 10 3	92.70
1.0574	1	12 7 1	93.52
1.0574	2	7 12 1	93.52
1.0559	2	10 4 4	93.68
1.0559	3	4 10 4	93.68
1.0526	2	10 10 0	94.08
1.0469	1	1 14 1	94.75
1.0467	1	3 8 5	94.77
1.0467	1	8 3 5	94.77
1.0434	2	11 6 3	95.17
1.0267	1	13 6 1	97.22
1.0267	1	6 13 1	97.22
1.0267	2	3 14 1	97.22

Structure
Monoclinic, $P2_1/c$ (14), Z=2 [Sasvari and Jeffrey, 1966]

Lattice parameters
a=8.59±0.05, b=14.40±0.03, c=8.75±0.05Å
β=129.6°±0.2° [ibid.]

Scattering factors
Mg^{+2}, Cl^-, O° [3.3.1A]

Thermal parameters
Isotropic: Mg 0.86; Cl 1.74; O(1) 2.12 O(2) 2.42; O(3) 1.81; O(4) 2.42; O(5) 2.03; O(6) 2.32

Density
(calculated) 1.241 g/cm³

Scale factor
1.198×10^4

Reference
Sasvari, K. and G.A. Jeffrey (1966). The crystal structure of magnesium chloride dodecahydrate, $MgCl_2 \cdot 12H_2O$, Acta Cryst. 20, 875-881.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
7.20	5	0	2	0		12.28
6.89	23	-1	1	1		12.84
6.61	20	1	0	0		13.38
6.10	47	0	1	1		14.50
6.01	34	1	1	0		14.72
5.30	2	-1	2	1		16.70
4.92	17	0	2	1		18.02
4.87	28	1	2	0		18.20
4.32	26	-1	0	2		20.56
4.09	100	-1	3	1		21.70
4.05	25	-2	1	1		21.94
3.92	61	-2	0	2	+	22.66
3.89	17	1	3	0		22.86
3.78	4	-2	1	2		23.50
3.70	17	-1	2	2		24.02
3.64	33	-2	2	1		24.44
3.60	8	0	4	0		24.72
3.58	50	1	1	1		24.88
3.44	46	-2	2	2		25.86
3.37	30	0	0	2		26.42
3.31	18	2	0	0		26.92
3.28	51	1	2	1	+	27.14
3.27	52	-1	4	1		27.22
3.22	4	2	1	0		27.64
3.21	9	-1	3	2		27.78
3.17	42	-2	3	1	+	28.14
3.05	31	0	2	2		29.22
3.04	21	-2	3	2		29.32
2.927	14	1	3	1		30.52
2.855	10	-2	1	3		31.30
2.808	6	-3	1	2		31.84
2.764	9	-1	4	2		32.36
2.738	4	-2	4	1		32.68
2.725	3	2	3	0		32.84
2.703	10	-1	5	1	+	33.12
2.673	2	-1	1	3		33.50
2.660	9	-3	2	2		33.66
2.653	6	0	5	1		33.76
2.612	1	-3	1	1		34.30
2.577	1	1	4	1		34.78
2.545	6	-1	2	3		35.24
2.491	1	-3	2	1		36.02
2.458	28	-3	3	2	+	36.52
2.400	13	0	6	0		37.44
2.395	16	-1	5	2		37.52
2.367	5	-1	3	3		37.98
2.324	21	-3	3	1	+	38.72
2.295	48	-3	3	3	+	39.22
2.271	23	1	5	1		39.66
2.261	29	0	6	1	+	39.84

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
2.220	18	0 1 3	40.60
2.207	2	3 0 0	40.86
2.180	17	3 1 0	41.38
2.175	30	1 3 2 +	41.48
2.162	8	2 3 1	41.74
2.158	15	-2 0 4 +	41.82
2.146	11	0 2 3	42.08
2.138	15	-3 4 1 +	42.24
2.115	4	-3 4 3	42.72
2.110	5	3 2 0 +	42.82
2.097	6	-1 6 2	43.10
2.087	12	-4 1 2 +	43.32
2.067	19	-2 2 4 +	43.76
2.047	8	-2 6 2 +	44.20
2.042	7	-4 2 3	44.32
2.036	4	0 3 3	44.46
2.025	9	-4 2 2	44.72
2.020	7	1 4 2	44.84
2.004	2	3 3 0	45.20
1.9779	4	-1 5 3	45.84
1.9641	3	1 7 0	46.18
1.9601	4	-4 0 4	46.28
1.9529	7	-3 5 1 +	46.46
1.9474	6	-4 3 3	46.60
1.9419	4	-1 1 4	46.74
1.9317	3	-4 3 2	47.00
1.8975	1	-4 1 1	47.90
1.8901	1	-1 2 4	48.10
1.8813	1	3 4 0	48.34
1.8617	3	1 5 2	48.88
1.8518	19	-2 6 3 +	49.16
1.8469	13	2 0 2	49.30
1.8309	3	2 1 2	49.76
1.8206	4	-4 4 2 +	50.06
1.7971	3	1 7 1	50.76
1.7879	1	2 2 2	51.04
1.7717	5	0 5 3 +	51.54
1.7546	1	-1 8 1	52.08
1.7391	2	0 8 1	52.58
1.7367	2	1 8 0	52.66
1.7209	5	-1 4 4 +	53.18
1.7025	2	-5 1 3	53.80
1.6903	6	1 3 3 +	54.22
1.6863	5	-5 0 4 +	54.36
1.6806	2	-2 7 3	54.56
1.6755	5	-5 1 4 +	54.74
1.6710	4	-3 7 2	54.90
1.6615	2	-1 8 2	55.24
1.6549	3	4 0 0	55.48
1.6429	5	-5 2 4 +	55.92

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.6402	4	0 6 3	56.02
1.6359	3	-2 8 2	56.18
1.6269	3	-5 1 2	56.52
1.6232	2	3 6 0	56.66
1.6164	2	-3 7 3 +	56.92
1.6071	1	-4 3 5	57.28
1.5878	3	0 8 2	58.04
1.5814	7	2 6 0	58.30
1.5739	2	-3 4 5	58.54
1.5681	3	2 7 1 +	58.84
1.5594	1	-5 1 5	59.20
1.5554	2	1 9 0	59.38
1.5410	2	-4 4 5	59.98
1.5299	2	1 5 3	60.46
1.5276	2	-5 4 4 +	60.56
1.5186	4	-4 6 4 +	60.96
1.5043	2	3 7 0	61.60
1.5004	2	-1 9 2	61.78
1.4951	3	-3 5 5 +	62.02
1.4912	5	-5 3 5 +	62.20
1.4831	2	-5 1 1	62.58
1.4797	2	-4 7 3	62.74
1.4734	4	-5 5 3	63.04
1.4680	3	1 9 1 +	63.30
1.4634	2	2 6 2	63.52
1.4593	2	3 1 2	63.72
1.4536	5	-1 3 5	64.00
1.4435	1	2 2 3	64.50
1.4379	1	-5 4 5	64.78
1.4274	2	-4 2 6	65.32
1.4231	4	1 1 4 +	65.54
1.4189	3	-1 7 4	65.76
1.4105	1	-3 2 6	66.20
1.4052	4	4 1 1	66.48
1.4015	4	-4 7 1 +	66.68
1.3967	2	-3 9 2	66.94
1.3949	2	3 8 0	67.04
1.3857	1	4 2 1	67.54
1.3821	3	-2 8 4	67.74
1.3786	2	-5 5 5 +	67.94
1.3746	2	-2 6 5	68.16
1.3693	2	-4 8 2	68.46
1.3655	1	-3 9 3	68.68

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
7.20	4	0 2 0	12.28
6.89	20	-1 1 1	12.84
6.62	17	1 0 0	13.37
6.11	40	0 1 1	14.49
6.01	28	1 1 0	14.72
5.30	2	-1 2 1	16.70
4.92	15	0 2 1	18.01
4.87	26	1 2 0	18.19
4.32	25	-1 0 2	20.56
4.13	2	-1 1 2	21.48
4.09	100	-1 3 1	21.69
4.05	22	-2 1 1	21.93
3.92	56	-2 0 2	22.66
3.91	11	0 3 1	22.72
3.89	14	1 3 0	22.87
3.78	3	-2 1 2	23.49
3.70	17	-1 2 2	24.02
3.64	33	-2 2 1	24.43
3.60	5	0 4 0	24.71
3.58	50	1 1 1	24.88
3.44	49	-2 2 2	25.85
3.37	30	0 0 2	26.42
3.31	16	2 0 0	26.92
3.28	44	1 2 1	27.13
3.28	8	0 1 2	27.15
3.27	36	-1 4 1	27.23
3.23	2	2 1 0	27.63
3.21	8	-1 3 2	27.77
3.18	19	0 4 1	28.08
3.17	26	-2 3 1	28.13
3.16	18	1 4 0	28.19
3.05	34	0 2 2	29.23
3.04	3	-2 3 2	29.39
2.926	16	1 3 1	30.53
2.863	1	-3 0 2	31.22
2.855	10	-2 1 3	31.31
2.808	6	-3 1 2	31.85
2.764	9	-1 4 2	32.36
2.739	4	-2 4 1	32.67
2.725	3	2 3 0	32.84
2.703	9	-1 5 1	33.11
2.700	3	-2 2 3	33.15
2.673	1	-1 1 3	33.49
2.660	10	-3 2 2	33.66
2.648	2	0 5 1	33.82
2.612	2	-3 1 1	34.30
2.577	1	1 4 1	34.78
2.545	7	-1 2 3	35.24
2.492	1	-3 2 1	36.01
2.461	1	0 4 2	36.49

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
2.459	24	-3 3 2	36.52
2.457	9	-3 2 3	36.54
2.406	4	1 1 2	37.35
2.400	10	0 6 0	37.44
2.396	12	-1 5 2	37.51
2.367	6	-1 3 3	37.99
2.324	24	-3 3 1	38.71
2.321	1	-2 5 2	38.76
2.296	43	-3 3 3	39.21
2.296	10	2 2 1	39.21
2.295	6	-1 6 1	39.22
2.271	25	1 5 1	39.66
2.264	2	-2 4 3	39.78
2.261	29	0 6 1	39.84
2.220	21	0 1 3	40.60
2.206	1	3 0 0	40.87
2.190	1	0 5 2	41.19
2.181	17	3 1 0	41.37
2.175	25	1 3 2	41.48
2.173	3	2 5 0	41.53
2.162	5	2 3 1	41.73
2.159	2	-3 0 4	41.81
2.158	13	-2 0 4	41.83
2.145	11	0 2 3	42.09
2.137	15	-3 4 1	42.25
2.135	2	-3 1 4	42.30
2.115	4	-3 4 3	42.71
2.110	1	-4 0 2	42.83
2.109	2	3 2 0	42.83
2.107	1	-4 1 3	42.88
2.097	7	-1 6 2	43.09
2.087	11	-4 1 2	43.31
2.086	3	-2 6 1	43.34
2.068	7	-3 2 4	43.74
2.067	17	-2 2 4	43.76
2.048	3	-2 5 3	44.19
2.047	6	-2 6 2	44.21
2.043	4	-4 2 3	44.31
2.035	3	0 3 3	44.48
2.025	11	-4 2 2	44.73
2.020	2	1 4 2	44.84
2.012	1	1 6 1	45.02
2.005	1	3 3 0	45.19
1.9776	5	-1 5 3	45.85
1.9644	2	1 7 0	46.17
1.9607	3	-4 0 4	46.27
1.9551	1	0 6 2	46.41
1.9525	7	-3 5 1	46.47
1.9469	3	-4 3 3	46.61
1.9412	2	-1 1 4	46.76

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.9314	3	-4	3	2	47.01
1.8973	1	-4	1	1	47.90
1.8904	2	-1	2	4	48.09
1.8811	1	3	4	0	48.35
1.8617	3	1	5	2	48.88
1.8521	19	-2	6	3	49.15
1.8513	1	-3	4	4	49.17
1.8508	5	-2	4	4	49.19
1.8498	1	-4	2	1	49.22
1.8491	4	-2	7	1	49.24
1.8456	3	2	0	2	49.34
1.8306	3	2	1	2	49.77
1.8217	2	-2	7	2	50.03
1.8202	4	-4	4	2	50.07
1.7969	3	1	7	1	50.77
1.7878	1	2	2	2	51.04
1.7734	1	3	1	1	51.49
1.7717	6	0	5	3	51.54
1.7544	2	-1	8	1	52.09
1.7391	2	0	8	1	52.58
1.7369	2	1	8	0	52.65
1.7219	1	-4	4	4	53.15
1.7208	5	-1	4	4	53.18
1.7026	3	-5	1	3	53.80
1.6905	6	1	3	3	54.22
1.6900	2	-4	4	1	54.23
1.6872	2	-5	0	4	54.33
1.6855	2	0	0	4	54.39
1.6803	1	-2	7	3	54.57
1.6757	5	-5	1	4	54.73
1.6747	3	3	3	1	54.77
1.6705	2	-3	7	2	54.92
1.6613	2	-1	8	2	55.25
1.6547	3	4	0	0	55.49
1.6439	2	4	1	0	55.88
1.6433	1	-3	3	5	55.91
1.6427	4	-5	2	4	55.93
1.6423	1	2	4	2	55.94
1.6404	2	0	6	3	56.01
1.6359	1	-2	8	2	56.18
1.6269	4	-5	1	2	56.52
1.6242	1	3	6	0	56.62
1.6166	2	-3	7	3	56.91
1.6144	1	1	4	3	57.00
1.6069	1	-4	3	5	57.29
1.5878	4	0	8	2	58.04
1.5812	10	2	8	0	58.31
1.5732	1	-3	4	5	58.63
1.5680	2	2	7	1	58.85
1.5677	1	-1	9	1	58.86

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.5593	1	-5	1	5	59.21
1.5552	2	1	9	0	59.38
1.5412	3	-4	4	5	59.97
1.5302	2	1	5	3	60.45
1.5277	2	-5	4	4	60.56
1.5265	1	0	4	4	60.61
1.5201	3	-2	4	5	60.89
1.5184	2	3	5	1	60.97
1.5164	3	-4	6	4	60.97
1.5046	2	3	7	0	61.59
1.5002	1	-1	9	2	61.79
1.4964	1	-4	6	1	61.96
1.4960	1	-2	9	1	61.98
1.4949	2	-3	5	5	62.03
1.4919	2	-1	2	5	62.17
1.4909	4	-5	3	5	62.21
1.4892	2	-3	7	4	62.30
1.4831	2	-5	1	1	62.58
1.4797	1	-4	7	3	62.74
1.4733	5	-5	5	3	63.04
1.4680	2	1	9	1	63.30
1.4674	2	-4	5	5	63.33
1.4630	2	2	6	2	63.54
1.4591	2	3	1	2	63.73
1.4534	7	-1	3	5	64.01
1.4433	1	2	2	3	64.51
1.4380	2	-5	4	5	64.78
1.4273	2	-4	2	6	65.32
1.4243	1	-6	1	4	65.48
1.4239	1	-5	3	1	65.50
1.4234	1	-5	5	2	65.52
1.4229	3	1	1	4	65.55
1.4187	2	-1	7	4	65.77
1.4107	1	-3	2	6	66.19
1.4082	1	0	10	1	66.32
1.4053	4	4	1	1	66.47
1.4023	1	-2	9	3	66.64
1.4013	2	-4	7	1	66.69
1.3966	2	-3	9	2	66.94
1.3947	2	3	8	0	67.05
1.3857	1	4	2	1	67.54
1.3822	3	-2	8	4	67.73
1.3775	1	-5	4	1	68.00
1.3775	1	-5	5	5	68.00
1.3746	2	-2	6	5	68.16
1.3693	2	-4	8	2	68.46
1.3647	1	-3	9	3	68.73

Structure

Orthorhombic, Pbca (61), Z=8 [Sutor, 1967]

Lattice parameters

a=10.215±0.002, b=10.681±0.002, c=10.014±0.002Å [ibid.]

Scattering factors

Mg^0, P^0, O^{-1} [3.3.1A]

Thermal parameters

Isotropic [Sutor, 1967]

Density

(calculated) 2.119 g/cm³ [ibid.]

Scale factor

4.210×10^4

Additional patterns

1. PDF card 19-762 [Cohen and Ribbe, 1966]
2. PDF card 19-763[Rassonskaya and Novikova,1965]

References

Cohen, L.H. and P.H. Ribbe (1966). Magnesium phosphate mineral replacement at Mono Lake, California, Am. Mineralogist 51, 1755-1765.

Rassonskaya, N.S. and O.S. Novikova(1965). Dehydration of magnesium hydrogen phosphate crystal hydrates, Russ. J. Inorg. Chem. 10, 774-776.

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Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.941	100	1 1 1	14.90
5.336	60	0 2 0	16.60
5.104	9	2 0 0	17.36
4.711	95	0 2 1	18.82
4.609	28	2 1 0	19.24
4.494	37	1 0 2	19.74
4.145	35	1 1 2	21.42
3.690	12	2 2 0	24.10
3.654	14	0 2 2	24.34
3.576	13	2 0 2	24.88
3.463	81	2 2 1	25.70
3.440	22	1 2 2	25.88
3.391	2	2 1 2	26.26
3.186	15	1 3 1	27.98
3.087	55	3 1 1	28.90
3.042	66	1 1 3	29.34
2.970	3	2 2 2	30.06
2.829	2	0 2 3	31.60
2.815	18	3 0 2	31.76
2.806	12	2 3 1	31.86
2.791	26	1 3 2	32.04
2.722	30	3 1 2	32.88
2.703	9	2 1 3	33.12
2.670	5	0 4 0	33.54
2.580	35	0 4 1	34.74
2.553	3	4 0 0	35.12
2.523	11	2 3 2	35.56
2.502	5	1 4 1	35.86
2.483	4	4 1 0	36.14
2.431	7	1 0 4	36.94
2.411	10	4 1 1	37.26
2.390	12	3 3 1	37.60
2.371	12	1 1 4 +	37.92
2.366	13	2 4 0	38.00
2.326	1	3 1 3	38.68
2.304	2	4 2 0	39.06
2.296	2	1 4 2	39.20
2.275	3	4 0 2	39.58
2.246	1	4 2 1	40.12
2.224	1	4 1 2	40.52
2.213	3	1 2 4	40.74
2.208	5	3 3 2	40.84
2.199	9	2 1 4 +	41.00
2.176	7	3 2 3	41.46
2.140	6	2 4 2	42.20
2.093	8	4 2 2	43.18
2.071	6	2 2 4	43.66
2.056	4	3 4 1	44.00
2.043	11	1 4 3	44.30
2.033	2	4 3 1	44.54

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.9812	6	3 1 4 +	45.76
1.9706	3	2 5 0	46.02
1.9673	2	5 1 1	46.10
1.9294	15	1 5 2 +	47.06
1.9171	1	4 3 2	47.38
1.9005	1	2 3 4	47.82
1.8960	4	4 2 3	47.94
1.8871	7	3 2 4	48.18
1.8747	8	5 2 1 +	48.52
1.8625	1	5 1 2	48.86
1.7978	10	1 4 4	50.74
1.7879	4	4 0 4	51.04
1.7717	1	1 5 3	51.54
1.7628	5	4 1 4	51.82
1.7603	5	2 2 5	51.90
1.7553	8	3 3 4 +	52.06
1.7318	2	4 4 2	52.82
1.7197	6	2 4 4 +	53.22
1.7025	2	6 0 0 +	53.80
1.6973	2	2 5 3	53.98
1.6812	12	2 6 0 +	54.54
1.6704	7	5 3 2 +	54.92
1.6576	6	2 6 1 +	55.38
1.6549	5	1 6 2 +	55.48
1.6386	6	4 5 0	56.08
1.6169	1	4 5 1	56.90
1.6122	1	6 0 2	57.08
1.6050	3	1 5 4	57.36
1.6009	5	6 2 1 +	57.52
1.5974	5	4 3 4	57.66
1.5935	5	0 2 6 +	57.82
1.5863	6	2 0 6	58.10
1.5826	5	5 0 4	58.24
1.5691	2	2 1 6	58.80
1.5657	6	5 1 4 +	58.94
1.5571	2	4 5 2	59.30

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.942	99	1 1 1	14.90
5.341	65	0 2 0	16.59
5.107	10	2 0 0	17.35
4.712	100	0 2 1	18.82
4.608	31	2 1 0	19.25
4.496	41	1 0 2	19.73
4.144	40	1 1 2	21.43
3.691	13	2 2 0	24.09
3.653	16	0 2 2	24.35
3.575	15	2 0 2	24.88
3.463	94	2 2 1	25.70
3.439	20	1 2 2	25.88
3.391	2	2 1 2	26.26
3.187	18	1 3 1	27.97
3.086	68	3 1 1	28.91
3.042	79	1 1 3	29.34
2.971	4	2 2 2	30.05
2.851	2	0 2 3	31.58
2.816	21	3 0 2	31.75
2.804	4	2 3 1	31.89
2.791	32	1 3 2	32.04
2.723	39	3 1 2	32.87
2.703	9	2 1 3	33.11
2.670	6	0 4 0	33.53
2.580	45	0 4 1	34.74
2.554	4	4 0 0	35.11
2.523	14	2 3 2	35.55
2.502	6	1 4 1	35.87
2.484	5	4 1 0	36.13
2.432	9	1 0 4	36.94
2.411	14	4 1 1	37.27
2.390	16	3 3 1	37.61
2.371	14	1 1 4	37.92
2.369	1	1 3 3	37.95
2.366	8	2 4 0	37.99
2.326	1	3 1 3	38.67
2.304	3	4 2 0	39.06
2.296	2	1 4 2	39.21
2.275	4	4 0 2	39.58
2.245	1	4 2 1	40.13
2.225	1	4 1 2	40.51
2.213	3	1 2 4	40.74
2.208	4	3 3 2	40.83
2.200	8	2 1 4	40.99
2.198	6	2 3 3	41.03
2.177	9	3 2 3	41.45
2.139	8	2 4 2	42.20
2.093	11	4 2 2	43.19
2.072	9	2 2 4	43.65
2.056	5	3 4 1	44.00

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
2.043	16	1	4	3	44.30
2.032	2	4	3	1	44.55
1.9820	6	3	1	4	45.74
1.9807	3	3	3	3	45.77
1.9708	3	2	5	0	46.02
1.9675	1	5	1	1	46.10
1.9375	2	3	4	2	46.85
1.9337	2	2	5	1	46.95
1.9329	4	1	1	5	46.97
1.9305	1	2	4	3	47.03
1.9295	18	1	5	2	47.06
1.9170	1	4	3	2	47.38
1.9008	1	2	3	4	47.81
1.8961	4	4	2	3	47.94
1.8869	10	3	2	4	48.19
1.8753	3	0	2	5	48.50
1.8744	10	5	2	1	48.53
1.8626	1	5	1	2	48.86
1.7978	15	1	4	4	50.74
1.7877	5	4	0	4	51.05
1.7720	1	1	5	3	51.53
1.7632	6	4	1	4	51.81
1.7604	5	2	2	5	51.90
1.7549	10	3	3	4	52.07
1.7527	1	0	6	1	52.14
1.7317	2	4	4	2	52.82
1.7198	4	5	1	3	53.22
1.7197	5	2	4	4	53.22

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
1.7042	1	3	1	5	53.74
1.7025	2	6	0	0	53.80
1.6971	1	2	5	3	53.99
1.6813	6	6	1	0	54.54
1.6810	12	2	6	0	54.55
1.6705	9	5	3	2	54.92
1.6690	1	0	0	6	54.97
1.6581	4	6	1	1	55.36
1.6578	4	2	6	1	55.37
1.6566	1	5	2	3	55.42
1.6551	5	1	6	2	55.47
1.6518	1	2	3	5	55.59
1.6385	9	4	5	0	56.08
1.6170	2	4	5	1	56.90
1.6119	1	6	0	2	57.09
1.6048	3	1	5	4	57.37
1.6022	1	0	4	5	57.47
1.6012	6	6	2	1	57.51
1.5976	3	4	3	4	57.65
1.5938	1	6	1	2	57.80
1.5930	6	0	2	6	57.83
1.5864	8	2	0	6	58.10
1.5828	3	5	0	4	58.24
1.5692	2	2	1	6	58.79
1.5657	8	5	1	4	58.94
1.5651	1	5	3	3	58.96
1.5573	2	4	5	2	59.29

Structure

Cubic, $I\bar{4}3m$ (217), Z=58 [Gazzara et al., 1967]

Lattice parameters

a=8.9129Å (published value: a=8.9125Å) [ibid.]

Scattering factors

Mn° [Freeman and Watson,1961], corrected for dispersion [Dauben and Templeton, 1955]

Thermal parameters

Isotropic [Gazzara et al., 1967]

Density

(calculated) 7.472 g/cm^3

Scale factor

62.21 x 10^4

Additional patterns

1. PDF 1-1237 [Hanawalt et al., 1938]

Reference

Dauben, C.H. and D.H. Templeton (1955). A table of dispersion corrections for x-ray scattering of atoms, Acta Cryst. **8**, 841-842.

Freeman, A.J. and R.E. Watson (1961). Hartree-Fock atomic scattering factors for the neutral atom iron transition series, Acta Cryst. **14**, 231-234.

Gazzara, C.P., R.M. Middleton, R.J. Weiss, and E.O.Hall (1967). A refinement of the parameters of α manganese,Acta Cryst.**22**, 859-862.

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-513.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
3.639	1	2 1 1	24.44
3.151	1	2 2 0	28.30
2.573	1	2 2 2	34.84
2.382	1	3 2 1	37.74
2.229	4	4 0 0	40.44
2.101	100	4 1 1 +	43.02
1.9005	21	3 3 2	47.82
1.8192	8	4 2 2	50.10
1.7478	12	4 3 1 +	52.30
1.6274	1	5 2 1	56.50
1.4857	1	4 4 2	62.46
1.4459	1	5 3 2	64.38
1.3436	1	6 2 2	69.96
1.2865	3	4 4 4	73.56
1.2604	4	5 5 0	75.34
1.2128	14	7 2 1 +	78.86
1.1909	2	6 4 2	80.60
1.1703	1	7 3 0	82.32
1.1320	2	6 5 1 +	85.76
1.0809	1	8 2 0	90.90
1.0653	1	6 5 3	92.62
1.0503	4	8 2 2 +	94.34
.9842	1	8 3 3	103.00
.9611	1	7 6 1 +	106.54
.9501	1	6 6 4	108.34
.9395	3	7 5 4 +	110.14
.9003	1	8 5 3 +	117.64
.8498	1	9 5 2 +	130.02
.8348	2	7 7 4 +	134.66
.8205	3	9 6 1 +	139.70
.8136	2	10 4 2	142.42
.8069	3	11 1 0 +	145.32
.7940	3	10 5 1 +	151.90

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
3.639	1	2	1	1	24.44
3.151	1	2	2	0	28.30
2.573	1	2	2	2	34.84
2.382	1	3	2	1	37.73
2.228	6	4	0	0	40.45
2.101	49	3	3	0	43.02
2.101	100	4	1	1	43.02
1.9002	35	3	3	2	47.83
1.8193	13	4	2	2	50.10
1.7480	16	4	3	1	52.29
1.7480	4	5	1	0	52.29
1.6273	1	5	2	1	56.51
1.5285	1	4	3	3	60.52
1.4855	1	4	4	2	62.47
1.4459	1	5	3	2	64.38
1.3437	3	6	2	2	69.96
1.3141	1	6	3	1	71.77
1.2865	7	4	4	4	73.56
1.2605	9	5	5	0	75.34
1.2129	19	7	2	1	78.85
1.2129	6	5	5	2	78.85
1.2129	6	6	3	3	78.85
1.1910	5	6	4	2	80.59
1.1703	3	7	3	0	82.32
1.1319	3	6	5	1	85.76
1.1319	2	7	3	2	85.76
1.0971	1	7	4	1	89.19
1.0808	2	8	2	0	90.90
1.0653	2	6	5	3	92.62
1.0504	6	8	2	2	94.33
1.0504	4	6	6	0	94.33
1.0361	1	8	3	1	96.05

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.0224	1	6	6	2	97.77
1.0092	1	7	5	2	99.51
.9843	3	8	3	3	103.00
.9725	1	8	4	2	104.76
.9611	1	9	2	1	106.54
.9611	2	7	6	1	106.54
.9611	1	6	5	5	106.54
.9501	2	6	6	4	108.33
.9395	3	8	5	1	110.15
.9395	1	9	3	0	110.15
.9395	4	7	5	4	110.15
.9193	1	7	6	3	113.84
.9003	3	8	5	3	117.64
.9003	1	9	4	1	117.64
.8825	1	10	1	1	121.58
.8740	1	8	6	2	123.61
.8657	1	9	4	3	125.69
.8576	1	10	2	2	127.83
.8498	1	10	3	1	130.03
.8498	3	9	5	2	130.03
.8348	5	7	7	4	134.66
.8348	3	8	5	5	134.66
.8205	12	9	6	1	139.70
.8205	1	10	3	3	139.70
.8136	9	10	4	2	142.42
.8069	2	9	5	4	145.33
.8069	3	8	7	3	145.33
.8069	6	11	1	0	145.33
.7940	5	11	2	1	151.91
.7940	7	9	6	3	151.91
.7940	7	10	5	1	151.91

Structure

Monoclinic, $P2_1/a$ (14), Z=2 [Braun and Lingafelter,1967]

Lattice parameters

a=10.672±0.002, b=13.064±0.002, c=7.998±0.001Å, β=98.09±0.01°
(published value, b=13.063) [ibid.]

Scattering factors

N°, O^{-1} [3.3.1A]; Pd°, C°[Berghuis et al., 1955]; H°[Stewart et al.,1965]

Thermal parameters

Isotropic:

Pd	2.71	O	3.34	N	2.87
C(1)	3.11	C(2)	2.97	C(3)	3.48
C(4)	4.28	C(5)	4.56	C(6)	3.91
C(7)	3.21	C(8)	3.79	C(9)	5.39
C(10)	6.01	C(11)	4.29	C(12)	6.31

H(4) through H(123) as given by Braun and Lingfelter [1967]

Density

(calculated) 1.465 g/cm³ [ibid.]

Scale factor

21.84×10^4

Reference

Berghuis, J., IJ. M. Haanapel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A. L. Veenendaal (1955). New calculations of atomic scattering factors,Acta Cryst. **8**, 478-483.

Braun,R.L. and E.C.Lingafelter (1967). The crystal structure of bis-(N-isopropyl-3-ethylsalicylaldiminato)palladium, Acta Cryst. **22**, 787-792.

Stewart, R.F., E.R.Davidson, and W.T.Simpson (1965). Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule, J. Chem. Phys. 42, 3175-3187.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
8.22	100	1	1	0		10.76
7.91	9	0	0	1		11.18
6.77	4	0	1	1		13.06
6.52	14	0	2	0		13.56
6.04	4	1	1	-1		14.66
5.41	16	1	1	1		16.36
5.28	4	2	0	0		16.78
5.03	2	0	2	1		17.60
4.71	2	2	0	-1	+	18.82
4.43	2	2	1	-1		20.02
4.40	8	1	2	1		20.18
4.11	3	2	2	0		21.62
3.96	5	0	0	2		22.44
3.94	6	2	1	1		22.54
3.82	10	2	2	-1	+	23.26
3.79	2	0	1	2		23.46
3.73	7	1	1	-2		23.84
3.67	2	1	3	-1		24.24
3.51	18	1	3	1		25.34
3.493	18	2	2	1		25.48
3.422	1	1	1	2		26.02
3.401	2	3	1	0		26.18
3.361	1	2	3	0		26.50
3.290	2	3	1	-1		27.08
3.266	1	0	4	0		27.28
3.019	2	0	4	1	+	29.56
2.998	1	2	3	1		29.78
2.982	4	3	1	1		29.94
2.974	3	2	0	2		30.02
2.902	2	1	3	-2		30.78
2.773	3	2	4	0	+	32.26
2.749	1	1	3	2		32.54
2.708	1	2	2	2		33.08
2.684	1	2	4	-1		33.36
2.639	1	0	0	3		33.94
2.598	1	1	1	-3		34.50
2.563	2	2	4	1		34.98
2.536	2	1	5	0		35.36
2.520	1	0	4	2		35.60
2.505	4	3	3	1		35.82
2.448	1	0	2	3		36.68
2.431	1	4	2	-1		36.94
2.423	1	3	1	2		37.08
2.393	1	1	5	1		37.56
2.356	2	4	0	-2		38.16
2.340	2	2	2	-3		38.44
2.258	1	4	2	1		39.90
2.237	2	3	1	-3		40.28
2.216	1	4	2	-2		40.68
2.198	1	2	4	2		41.02

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.177	1	0 6 0	41.44
2.155	1	1 3 3	41.88
2.146	1	3 3 2	42.08
2.118	1	2 2 3	42.66
2.104	1	1 5 2	42.96
2.099	2	0 6 1 +	43.06
2.014	2	3 3 -3 +	44.98
1.9746	1	1 1 -4	45.92
1.9706	1	4 2 2	46.02
1.9609	1	5 1 -2	46.26
1.9248	1	4 2 -3	47.18
1.9043	1	5 3 -1	47.72
1.8646	1	2 2 -4	48.80
1.7998	1	1 7 -1	50.68
1.7932	1	3 5 2	50.88
1.7465	1	4 4 2	52.34

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
8.22	100	1 1 0	10.76
7.92	9	0 0 1	11.16
6.77	5	0 1 1	13.06
6.53	15	0 2 0	13.54
6.04	4	1 1 -1	14.65
5.41	19	1 1 1	16.36
5.28	5	2 0 0	16.77
5.04	3	0 2 1	17.59
4.72	1	1 2 -1	18.80
4.71	2	2 0 -1	18.82
4.43	1	2 1 -1	20.02
4.40	9	1 2 1	20.18
4.11	3	2 2 0	21.62
3.96	6	0 0 2	22.44
3.94	5	2 1 1	22.54
3.82	11	2 2 -1	23.26
3.82	1	0 3 1	23.29
3.79	1	0 1 2	23.46
3.73	9	1 1 -2	23.84
3.67	2	1 3 -1	24.24
3.51	23	1 3 1	25.33
3.493	20	2 2 1	25.48
3.423	1	1 1 2	26.01
3.401	3	3 1 0	26.18
3.360	2	2 3 0	26.50
3.291	2	3 1 -1	27.07
3.266	1	0 4 0	27.28

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.021	1	2 2 -2	29.55
3.019	1	0 4 1	29.56
2.996	1	2 3 1	29.77
2.981	5	3 1 1	29.95
2.974	1	2 0 2	30.02
2.902	3	1 3 -2	30.79
2.778	2	2 4 0	32.20
2.773	2	3 1 -2	32.26
2.772	1	3 2 1	32.26
2.750	2	1 3 2	32.53
2.706	2	2 2 2	33.07
2.684	1	2 4 -1	33.35
2.639	2	0 0 3	33.94
2.597	2	1 1 -3	34.51
2.563	2	2 4 1	34.98
2.536	2	1 5 0	35.36
2.519	1	0 4 2	35.61
2.505	5	3 3 1	35.82
2.447	1	0 2 3	36.69
2.431	1	4 2 -1	36.95
2.422	1	3 1 2	37.09
2.392	2	1 5 1	37.57
2.377	1	3 3 -2	37.81
2.356	2	4 0 -2	38.17
2.340	2	2 2 -3	38.44
2.258	1	4 2 1	39.90
2.238	3	3 1 -3	40.27
2.216	1	4 2 -2	40.66
2.199	2	2 4 2	41.01
2.177	2	0 6 0	41.44
2.155	1	1 3 3	41.89
2.145	1	3 3 2	42.09
2.116	1	2 2 3	42.66
2.104	1	1 5 2	42.96
2.099	2	0 6 1	43.05
2.098	1	3 5 0	43.07
2.014	1	3 3 -3	44.98
2.013	1	2 6 0	44.99
1.9743	1	1 1 -4	45.93
1.9706	1	4 2 2	46.01
1.9613	1	5 1 -2	46.25
1.9372	1	4 4 1	46.86
1.9247	1	4 2 -3	47.18
1.9041	1	5 3 -1	47.72
1.8649	1	2 2 -4	48.79
1.8000	1	1 7 -1	50.67
1.7929	1	3 5 2	50.89
1.7807	1	1 7 1	51.26
1.7467	1	4 4 2	52.34
1.6717	1	2 4 -4	54.88

Structure
Triclinic, $P\bar{1}$ (2), Z=1 [Fritchie,1966]

Lattice parameters
a= 3.8684±0.0004Å, α=91.67°±0.01°
b= 7.7810±0.0008, β=92.67°±0.01°
c=15.736 ±0.002, γ=95.38°±0.01° at 23°C
(published values: a=3.8682, b=7.7807, c=15.735Å) [ibid.]

Scattering factors
H^0, C^0, N^0 [3.3.1A]

Thermal parameters
Anisotropic for carbon and nitrogen, isotropic for hydrogen [Fritchie,1966]

Density
(calculated) 1.4090 g/cm³ [ibid.]

Scale factor
0.9160 × 10^4

Reference
Fritchie, C.J.Jr.(1966).The crystal structure of N-methylphenazinium tetracyanoquinodimethanide, Acta Cryst.20 892-898.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
7.85	16	0 0 2	11.26
7.74	13	0 1 0	11.42
7.03	33	0 -1 1	12.58
6.85	100	0 1 1	12.92
5.60	11	0 -1 2	15.80
5.42	5	0 1 2	16.34
4.41	1	0 -1 3	20.14
3.87	2	0 2 0	22.96
3.85	3	1 0 0	23.10
3.78	9	-1 0 1	23.52
3.73	2	0 2 1	23.84
3.69	2	1 0 1	24.08
3.55	6	0 -1 4	25.06
3.52	7	-1 0 2 +	25.30
3.471	8	1 -1 1	25.64
3.427	2	0 2 2	25.98
3.297	7	-1 1 2	27.02
3.288	6	-1 -1 1	27.10
3.222	5	1 -1 2	27.66
3.213	4	1 1 1	27.74
3.175	61	-1 0 3	28.08
3.142	8	0 0 5	28.38
3.123	43	-1 -1 2	28.56
3.064	2	0 2 3	29.12
3.029	1	1 0 3	29.46
2.945	3	0 -1 5	30.32
2.827	3	-1 2 1	31.62
2.820	3	-1 0 4	31.70
2.805	1	0 -2 4	31.88
2.735	2	1 1 3	32.72
2.608	2	1 -1 4	34.36
2.560	5	0 -3 1	35.02
2.534	1	0 3 1	35.40
2.503	1	1 -2 3	35.84
2.477	1	0 -3 2	36.24
2.468	3	1 1 4	36.38
2.377	1	1 0 5	37.82
2.204	1	0 -2 6	40.92
2.157	2	-1 3 2	41.84
2.136	2	0 1 7 +	42.28
2.106	1	1 -2 5	42.90
1.9529	1	1 2 5	46.46
1.7853	1	-1 4 1	51.12
1.7622	1	-2 0 4	51.84
1.6179	2	-2 -1 5	56.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.85	14	0 0 2	11.26
7.74	11	0 1 0	11.42
7.04	32	0 -1 1	12.56
6.85	100	0 1 1	12.91
5.61	11	0 -1 2	15.79
5.42	6	0 1 2	16.33
4.41	1	0 -1 3	20.13
3.87	2	0 2 0	22.95
3.85	3	1 0 0	23.10
3.78	10	-1 0 1	23.52
3.73	3	0 2 1	23.84
3.69	2	1 0 1	24.07
3.55	6	0 -1 4	25.05
3.52	4	-1 0 2	25.25
3.52	2	0 -2 2	25.28
3.52	3	-1 1 1	25.30
3.471	3	1 -1 1	25.64
3.456	2	0 1 4	25.76
3.427	2	0 2 2	25.98
3.299	8	-1 1 2	27.01
3.288	3	-1 -1 1	27.10
3.223	5	1 -1 2	27.65
3.212	2	1 1 1	27.75
3.176	78	-1 0 3	28.07
3.142	6	0 0 5	28.38
3.124	53	-1 -1 2	28.55

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.064	2	0 2 3	29.12
3.029	1	1 0 3	29.46
2.946	3	0 -1 5	30.31
2.828	4	-1 2 1	31.61
2.819	1	-1 0 4	31.72
2.805	1	0 -2 4	31.88
2.735	3	1 1 3	32.72
2.608	2	1 -1 4	34.36
2.560	7	0 -3 1	35.02
2.533	1	0 3 1	35.41
2.503	1	1 -2 3	35.84
2.477	1	0 -3 2	36.24
2.457	4	1 1 4	36.38
2.376	1	1 0 5	37.83
2.204	2	0 -2 6	40.92
2.158	3	-1 3 2	41.83
2.136	3	0 1 7	42.27
2.136	1	0 2 6	42.28
2.106	1	1 -2 5	42.91
2.084	1	1 -1 6	43.38
1.9531	1	1 2 5	46.45
1.9355	1	0 4 0	46.90
1.8617	1	-1 -3 4	48.88
1.7859	1	-1 4 1	51.10
1.7521	1	-2 0 4	51.84
1.6181	3	-2 -1 5	56.85

Structure

Tetragonal, $P4_2/mnm(136)$, Z=4, [Sands, et al., 1959]

Lattice parameters

a=10.87±0.01Å, c=3.96±0.01Å [ibid.]

Scattering factors

Cl^{-1}, O^{-1} [3.3.1A]
Nb^{0} [3.3.1B]

Thermal parameters

Isotropic [Sands et al., 1959]

Density

(calculated) 3.04 g/cm³ [ibid.]

Scale factor

7.198×10^4

Reference

Sands, D.E., A. Zalkin, and R.E. Elson (1959). The crystal structure of $NbOCl_3$, Acta Cryst. 12, 21-23.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
7.69	80	1	1	0		11.50
4.86	100	2	1	0		18.24
3.72	83	1	0	1		23.90
3.52	36	1	1	1		25.28
3.44	7	3	1	0		25.90
3.07	2	2	1	1		29.06
3.02	1	3	2	0		29.60
2.758	1	2	2	1		32.44
2.717	59	4	0	0		32.94
2.673	9	3	0	1		33.50
2.636	2	4	1	0		33.98
2.596	11	3	1	1		34.52
2.562	2	3	3	0		35.00
2.399	1	3	2	1		37.46
2.194	17	4	1	1		41.10
2.132	3	5	1	0		42.36
2.019	9	5	2	0		44.86
1.9803	10	0	0	2		45.78
1.9217	11	4	4	0		47.26
1.9171	8	1	1	2		47.38
1.9056	15	5	0	1	+	47.68
1.8769	6	5	1	1		48.46
1.8639	1	5	3	0		48.82
1.8336	6	2	1	2		49.68
1.7873	4	6	1	0		51.06
1.7155	1	3	1	2		53.36
1.6869	3	5	3	1		54.34
1.6206	1	6	3	0		56.76
1.6004	11	4	0	2		57.54
1.5764	1	6	2	1		58.50
1.5604	7	5	4	1		59.16
1.5373	2	5	5	0	+	60.14
1.4507	2	5	1	2		64.14
1.4467	1	7	0	1		64.34
1.4332	1	5	5	1		65.02
1.4274	1	7	3	0		65.32
1.4135	3	5	2	2		66.04
1.3919	1	6	5	0		67.20
1.3789	4	4	4	2		67.92
1.3586	1	8	0	0	+	69.08
1.3265	2	6	1	2		71.00
1.3105	1	1	0	3		72.00
1.2764	1	7	4	1	+	74.24
1.2151	1	8	4	0		78.68
1.2143	2	5	5	2		78.74
1.1803	1	4	1	3		81.48
1.1791	1	9	2	0		81.58
1.1552	1	9	0	1		83.64
1.1386	1	6	5	2		85.14
1.1284	1	5	0	3		86.10

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
7.69	79	1 1 0	11.50
4.86	100	2 1 0	18.23
3.72	90	1 0 1	23.90
3.52	39	1 1 1	25.28
3.44	7	3 1 0	25.90
3.07	3	2 1 1	29.06
3.02	1	3 2 0	29.61
2.758	1	2 2 1	32.44
2.717	72	4 0 0	32.93
2.673	10	3 0 1	33.49
2.636	2	4 1 0	33.98
2.596	13	3 1 1	34.52
2.562	2	3 3 0	34.99
2.399	1	3 2 1	37.46
2.195	22	4 1 1	41.10
2.132	11	5 1 0	42.36
2.019	13	5 2 0	44.87
1.9800	14	0 0 2	45.79
1.9216	14	4 4 0	47.26
1.9174	3	1 1 2	47.37
1.9057	19	5 0 1	47.68
1.9057	5	4 3 1	47.68
1.8771	9	5 1 1	48.46
1.8642	2	5 3 0	48.81
1.8337	9	2 1 2	49.68
1.7870	6	6 1 0	51.07
1.7157	2	3 1 2	53.35
1.6866	5	5 3 1	54.35
1.6288	1	6 1 1	56.45
1.6204	2	6 3 0	56.77
1.6003	16	4 0 2	57.55
1.5766	2	6 2 1	58.49
1.5603	11	5 4 1	59.17
1.5372	1	7 1 0	60.14
1.5372	3	5 5 0	60.14
1.4997	1	6 3 1	61.81
1.4508	4	5 1 2	64.14
1.4457	1	7 0 1	64.39
1.4331	1	5 5 1	65.03
1.4273	1	7 3 0	65.32

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.4135	5	5 2 2	66.04
1.3918	2	6 5 0	67.21
1.3789	6	4 4 2	67.92
1.3587	2	8 0 0	69.07
1.3573	1	5 3 2	69.15
1.3266	3	6 1 2	70.99
1.3104	2	1 0 3	72.01
1.3009	1	1 1 3	72.61
1.2763	1	8 1 1	74.24
1.2763	1	7 4 1	74.24
1.2540	1	6 3 2	75.80
1.2188	1	6 6 1	78.39
1.2153	2	8 4 0	78.66
1.2142	2	5 5 2	78.75
1.2038	1	7 5 1	79.56
1.2004	1	9 1 0	79.84
1.1803	1	4 1 3	81.48
1.1790	1	9 2 0	81.59
1.1552	2	9 0 1	83.64
1.1386	2	6 5 2	85.14
1.1283	2	5 0 3	86.11
1.1223	1	5 1 3	86.68
1.1203	1	8 0 2	86.87
1.0632	2	9 4 1	92.86
1.0558	1	9 5 0	93.70
1.0420	2	5 4 3	95.33
1.0358	1	8 4 2	96.09
1.0293	1	10 2 1	96.90
1.0265	1	9 1 2	97.25
1.0130	1	9 2 2	99.00
.9492	1	10 1 2	108.48
.9316	1	9 5 2	111.55
.9302	1	4 0 4	111.80
.9073	1	10 6 1	116.20
.8911	1	9 0 3	119.64
.8801	1	4 4 4	122.15
.8467	1	9 4 3	130.94
.7842	1	9 9 2	158.38
.7834	1	11 8 1	159.01

Structure

Orthorhombic, Pnma(62),Z=4 [Breneman and Willett, 1967]

Lattice parameters

a=9.35±0.02, b=7.94±0.01, c=14.69±0.02Å [ibid.]

Scattering factors

P°, Br° [3.3.1A]

Thermal parameters

Isotropic: P .90; Br(1) 2.01;Br(2) 2.71; Br(3) 2.73; Br(4) 2.57; Br(5) 1.90; Br(6) 3.58

Density

(calculated) 3.60 g/cm^3 [Breneman and Willett, 1967]

Scale factor

37.67 × 10^4

Reference

Breneman, G.L. and R.D.Willett (1967). The crystal structure of phosphorus heptabromide, PBr_7, Acta Cryst. 23, 467-471.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.99	3	0 1 1	12.66
5.77	4	1 0 2	15.34
5.60	2	1 1 1	15.82
4.67	15	1 1 2 +	18.98
4.45	3	2 0 1	19.92
4.34	7	1 0 3	20.46
4.17	2	0 1 3	21.30
4.03	17	2 1 0	22.04
3.97	51	0 2 0	22.38
3.88	6	2 1 1	22.88
3.80	37	1 1 3	23.36
3.67	10	0 0 4	24.22
3.53	18	2 1 2	25.20
3.49	2	0 2 2	25.48
3.42	7	1 0 4	26.04
3.27	100	1 2 2	27.24
3.14	48	1 1 4	28.40
3.03	33	2 2 0	29.50
2.928	3	1 2 3	30.50
2.888	31	2 0 4	30.94

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.870	26	3 0 2	31.14
2.847	27	3 1 1	31.40
2.803	6	1 0 5	31.90
2.714	23	2 1 4	32.98
2.698	15	3 1 2 +	33.18
2.644	4	1 1 5	33.88
2.605	1	0 3 1	34.40
2.574	2	2 2 3	34.82
2.509	4	1 3 1	35.76
2.495	5	3 1 3	35.96
2.487	7	2 0 5	36.08
2.417	1	3 2 1	37.16
2.406	1	1 3 2	37.34
2.368	5	1 0 6	37.96
2.326	2	3 2 2 +	38.68
2.309	2	4 0 1	38.98
2.303	3	2 3 0	39.08
2.290	3	1 2 5	39.32
2.275	7	2 3 1	39.58
2.270	10	1 1 6	39.68
2.260	3	1 3 3	39.86
2.242	9	4 1 0	40.18
2.197	4	2 3 2	41.04
2.169	2	2 0 6	41.60
2.145	1	4 1 2	42.10
2.108	10	4 0 3 +	42.86
2.092	19	1 3 4 +	43.20
2.086	12	2 3 3 +	43.34
2.047	2	1 0 7	44.20
2.039	6	3 2 4	44.40
2.034	6	1 2 6	44.50
2.015	15	4 2 0	44.96
1.9985	2	3 3 1	45.34
1.9853	16	0 4 0 +	45.66
1.9722	3	4 0 4	45.98
1.9513	8	2 3 4	46.50
1.9458	5	3 3 2	46.64
1.9141	2	2 0 7 +	47.46
1.9035	1	2 2 6	47.74
1.8820	3	3 2 5	48.32
1.8711	2	3 1 6	48.62
1.8653	4	3 3 3 +	48.78
1.8199	2	1 2 7	50.08
1.8125	2	5 0 2	50.30
1.8064	2	5 1 1 +	50.48
1.7654	3	4 2 4 +	51.74
1.7571	3	1 1 8	52.00
1.7521	5	4 3 0	52.16
1.7471	3	5 0 3 +	52.32
1.7324	10	3 2 6	52.80

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.7167	1	1 4 4	53.32
1.7090	2	2 0 8	53.58
1.6909	1	4 0 6	54.20
1.6806	2	5 2 1	54.56
1.6777	4	2 3 6	54.66
1.6665	2	5 0 4	55.06
1.6626	2	3 3 5	55.20
1.6538	2	4 1 6	55.52
1.6489	4	5 2 2 +	55.70
1.6407	7	1 2 8	56.00
1.6359	7	2 4 4	56.18
1.6316	7	3 4 2 +	56.34
1.6200	2	1 4 5	56.78
1.5989	4	5 2 3 +	57.60
1.5819	5	3 0 8	58.28
1.5580	3	6 0 0 +	59.26
1.5514	4	2 3 7 +	59.54
1.5208	2	6 1 1 +	60.86
1.5190	3	5 3 1	60.94
1.5039	1	2 5 0	61.62
1.4908	3	1 5 3 +	62.22
1.4861	2	5 0 6	62.44
1.4692	3	0 0 10 +	63.24
1.4659	4	5 2 5	63.40
1.4597	1	6 1 3	63.70
1.4455	2	4 4 3 +	64.40
1.4403	2	1 5 4	64.66
1.4250	1	4 3 6	65.44
1.4212	1	3 1 9	65.64
1.4101	2	5 3 4	66.22
1.4082	3	3 5 1	66.32
1.3916	1	2 5 4	67.22
1.3894	2	3 5 2	67.34
1.3818	2	1 5 5	67.76
1.3490	3	6 2 4	69.64
1.3453	2	4 3 7	69.86
1.3232	1	0 6 0	71.20
1.3216	2	2 2 10	71.30
1.3184	1	1 5 6	71.50
1.3171	1	0 1 11	71.58
1.2953	1	2 4 8	72.98
1.2925	1	5 1 8	73.16
1.2898	1	1 6 2	73.34
1.2814	1	2 5 6	73.90
1.2602	1	3 2 10	75.36
1.2442	1	5 2 8	76.50
1.2398	1	7 1 4	76.82
1.2371	3	3 4 8 +	77.02
1.2256	2	6 4 0	77.88

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.98	2	0 1 1	12.66
5.78	3	1 0 2	15.33
5.60	1	1 1 1	15.82
4.68	3	2 0 0	18.97
4.67	11	1 1 2	18.98
4.45	2	2 0 1	19.91
4.34	7	1 0 3	20.46
4.17	1	0 1 3	21.30
4.03	15	2 1 0	22.05
3.97	47	0 2 0	22.38
3.94	2	2 0 2	22.53
3.89	6	2 1 1	22.87
3.81	37	1 1 3	23.35
3.67	10	0 0 4	24.21
3.55	2	1 2 1	25.09
3.53	17	2 1 2	25.19
3.49	2	0 2 2	25.48
3.42	7	1 0 4	26.05
3.27	100	1 2 2	27.23
3.14	49	1 1 4	28.40
3.03	34	2 2 0	29.49
2.929	3	1 2 3	30.50
2.888	31	2 0 4	30.94
2.869	26	3 0 2	31.15
2.846	27	3 1 1	31.40
2.803	5	1 0 5	31.90
2.714	24	2 1 4	32.98
2.698	9	3 1 2	33.17
2.696	8	0 2 4	33.20
2.643	5	1 1 5	33.89
2.605	1	0 3 1	34.40
2.574	2	2 2 3	34.82
2.509	4	1 3 1	35.76
2.496	4	3 1 3	35.95
2.488	7	2 0 5	36.08
2.418	2	3 2 1	37.15
2.406	1	1 3 2	37.34
2.368	5	1 0 6	37.96
2.328	1	0 3 3	38.64
2.325	2	3 2 2	38.69
2.308	2	4 0 1	38.98
2.303	2	2 3 0	39.08
2.290	3	1 2 5	39.32
2.275	7	2 3 1	39.57
2.270	7	1 1 6	39.68
2.259	3	1 3 3	39.87
2.242	10	4 1 0	40.18
2.198	4	2 3 2	41.04
2.169	2	2 0 6	41.60
2.145	2	4 1 2	42.10

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
2.109	7	4	0	3	42.83
2.108	6	2	2	5	42.87
2.093	12	1	3	4	43.19
2.092	10	2	1	6	43.20
2.084	5	2	3	3	43.38
2.084	2	0	2	6	43.39
2.048	2	1	0	7	44.19
2.039	6	3	2	4	44.39
2.034	4	1	2	6	44.51
2.014	18	4	2	0	44.97
1.9986	2	3	3	1	45.34
1.9850	19	0	4	0	45.67
1.9828	1	1	1	7	45.72
1.9719	3	4	0	4	45.99
1.9512	9	2	3	4	46.50
1.9453	1	3	3	2	46.65
1.9145	1	2	0	7	47.45
1.9138	1	4	1	4	47.47
1.9034	1	2	2	6	47.74
1.8823	3	3	2	5	48.31
1.8711	2	3	1	6	48.62
1.8653	4	3	3	3	48.78
1.8628	2	4	2	3	48.85
1.8198	2	1	2	7	50.08
1.8122	2	5	0	2	50.31
1.8064	2	5	1	1	50.48
1.8050	1	1	4	3	50.52
1.7661	2	4	2	4	51.72
1.7649	2	1	3	6	51.75
1.7571	2	1	1	8	52.00
1.7520	5	4	3	0	52.16
1.7469	1	5	0	3	52.33
1.7462	1	0	4	4	52.35
1.7323	12	3	2	6	52.80
1.7166	1	1	4	4	53.32
1.7091	3	2	0	8	53.58
1.6907	1	4	0	6	54.21
1.6806	2	5	2	1	54.56
1.6776	5	2	3	6	54.67
1.6664	1	5	0	4	55.06
1.6631	1	3	3	5	55.18
1.6536	2	4	1	6	55.53
1.6496	2	4	3	3	55.67
1.6486	3	5	2	2	55.71
1.6407	8	1	2	8	56.00
1.6358	5	2	4	4	56.18
1.6324	4	3	4	2	56.31
1.6309	4	5	1	4	56.37
1.6199	1	1	4	5	56.78
1.5990	3	5	2	3	57.60

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.5988	1	0	1	9	57.60
1.5821	7	3	0	8	58.27
1.5583	4	6	0	0	59.25
1.5568	1	1	5	1	59.31
1.5516	2	2	4	5	59.53
1.5512	3	2	3	7	59.55
1.5496	1	6	0	1	59.61
1.5213	1	1	4	6	60.84
1.5209	1	6	1	1	60.86
1.5191	3	5	3	1	60.94
1.5036	1	2	5	0	61.63
1.4912	3	1	5	3	62.20
1.4903	2	1	2	9	62.24
1.4894	1	1	3	8	62.28
1.4861	1	5	0	6	62.44
1.4697	1	3	2	8	63.22
1.4690	2	0	0	10	63.25
1.4660	4	5	2	5	63.39
1.4596	1	5	1	3	63.70
1.4456	3	4	4	3	64.40
1.4440	1	4	0	8	64.48
1.4402	3	1	5	4	64.67
1.4248	1	4	3	6	65.45
1.4225	1	3	1	9	65.57
1.4102	3	5	3	4	66.22
1.4084	4	3	5	1	66.31
1.3990	1	4	4	4	66.82
1.3915	1	2	5	4	67.22
1.3894	1	3	5	2	67.34
1.3817	2	1	5	5	67.77
1.3491	4	5	2	4	69.63
1.3449	1	4	3	7	69.88
1.3233	1	0	6	0	71.19
1.3215	2	2	2	10	71.31
1.3190	1	1	5	6	71.46
1.3170	1	0	1	11	71.59
1.2952	1	2	4	8	72.99
1.2927	1	5	1	8	73.15
1.2899	1	1	6	2	73.33
1.2813	1	2	5	6	73.91
1.2601	2	3	2	10	75.37
1.2442	1	5	2	8	76.50
1.2399	1	7	1	4	76.82
1.2372	4	3	4	8	77.01
1.2359	1	6	1	7	77.11
1.2257	2	6	4	0	77.87

Structure
Monoclinic, $P2_1/c$ (14), Z=4 [Housty and Hospital, 1966]

Lattice parameters
a=5.65±0.01, b=9.68±0.02, c=22.33±0.05Å
β=137° [ibid.]

Scattering factors
H^0, C^0, O^0 [3.3.1A]

Atomic positions
Table 1 [Housty and Hospital, 1966]

Thermal parameters
Isotropic: B=4.0Å² for carbon and oxygen
B=3.0Å² for hydrogen

Density
(calculated) 1.275 g/cm³ [ibid.]

Scale factor
2.867 x.10^4

Polymorphism
The existence of a second polymorph has been reported by Dupré la Tour [1935].

Additional patterns

1. PDF card 9-721[Whitney and Corvin,1949] It may represent a different polymorph.

Reference

Dupré la Tour, F.(1935).Polymorphisme dans la série des diacides gras normaux, Compt. Rend. 201, 479-481.

Housty, J. and M. Hospital (1966). Localisation des atomes d'hydrogène dans l'acide pimélique, COOH-$[CH_2]_5$-COOH, Acta Cryst. 21, 29-34.

Whitney, J. and I. Corvin (1949). Pimelic acid, Anal. Chem. 21, 191-192.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.61	36	0 0 2	11.62
5.98	2	0 1 2	14.80
5.22	1	-1 0 4	16.96
4.84	28	0 2 0	18.32
4.69	2	-1 1 2	18.90
4.61	74	0 2 1	19.22
4.08	1	0 2 2	21.74
3.85	100	1 0 0	23.06
3.70	5	-1 0 6	24.02
3.67	8	-1 2 3	24.20
3.59	4	-1 2 2	24.76
3.50	1	0 2 3	25.40
3.343	62	-1 2 1	26.64
3.276	3	-1 2 5	27.20
3.157	2	0 3 1	28.24
3.054	12	1 1 1	29.22
3.015	4	1 2 0	29.60
2.992	2	0 2 4	29.84
2.940	5	-1 2 6	30.38
2.822	3	-2 0 6	31.68
2.801	2	-1 3 3	31.92
2.764	5	-1 3 2	32.36
2.744	3	-1 3 4	32.60
2.711	1	-2 1 6	33.02
2.647	2	-1 3 1	33.84
2.612	7	-2 0 8 +	34.30
2.438	1	-2 2 6	36.84
2.431	2	-1 3 6	36.94
2.420	1	0 4 0	37.12
2.353	1	-2 1 9	38.22
2.314	8	-1 2 8 +	38.88
2.299	10	-2 2 8	39.16
2.285	2	1 1 3	39.40
2.248	1	0 2 6	40.08
2.224	1	-2 0 10	40.52
2.219	2	-1 1 9	40.62
2.206	1	-1 4 2	40.88
2.168	1	-2 2 9	41.62
2.113	1	-2 3 5	42.76
2.063	2	-1 2 9 +	43.84
2.042	1	0 4 4	44.32
2.021	1	-2 2 10	44.80
1.9372	3	-2 2 1	46.86
1.9263	1	2 0 0	47.14
1.8511	1	-1 2 10	49.18
1.8111	1	-3 1 7	50.34
1.7827	1	-1 4 8	51.20
1.7293	2	2 1 1	52.90
1.7131	2	-2 4 9	53.44
1.6671	1	0 1 9	55.04
1.6598	1	-1 4 9	55.30

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.61	29	0 0 2	11.61
5.98	2	0 1 2	14.79
5.22	1	-1 0 4	16.96
4.84	26	0 2 0	18.31
4.69	1	-1 1 2	18.90
4.61	73	0 2 1	19.23
4.08	1	0 2 2	21.74
3.85	100	1 0 0	23.06
3.70	5	-1 0 6	24.03
3.67	7	-1 2 3	24.20
3.59	4	-1 2 2	24.75
3.50	1	0 2 3	25.41
3.344	65	-1 2 1	26.63
3.276	3	-1 2 5	27.20
3.157	2	0 3 1	28.25
3.053	13	1 1 1	29.22
3.015	4	1 2 0	29.61
2.992	2	0 2 4	29.83
2.940	6	-1 2 6	30.38
2.823	3	-2 0 6	31.67
2.801	2	-1 3 3	31.92
2.765	6	-1 3 2	32.35
2.745	3	-1 3 4	32.59
2.710	1	-2 1 6	33.03
2.646	2	-1 3 1	33.84
2.612	7	-2 0 8	34.30
2.610	1	-1 2 7	34.33
2.438	2	-2 2 6	36.83

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.432	1	-1 3 6	36.93
2.420	1	0 4 0	37.12
2.353	1	-2 1 9	38.22
2.315	9	-1 2 8	38.87
2.313	1	-2 0 2	38.91
2.299	11	-2 2 8	39.15
2.285	2	1 1 3	39.41
2.248	1	0 2 6	40.08
2.225	1	-2 0 10	40.52
2.220	1	-1 1 9	40.61
2.206	1	-1 4 2	40.87
2.168	1	-2 2 9	41.61
2.113	1	-2 3 5	42.76
2.065	1	-2 1 1	43.81
2.063	2	-1 2 9	43.85
2.042	1	0 4 4	44.32
2.021	1	-2 2 10	44.80
1.9369	3	-2 2 1	46.87
1.9265	1	2 0 0	47.13
1.8507	1	-1 2 10	49.19
1.8117	1	-3 1 7	50.32
1.7968	1	-2 4 4	50.77
1.7827	1	-1 4 8	51.20
1.7297	2	2 1 1	52.89
1.7131	2	-2 4 9	53.44
1.6568	1	0 1 9	55.05
1.6597	1	-1 4 9	55.30

Structure
Monoclinic, $P2_1/n(14)$, Z=4, [Boonstra, 1968]

Lattice parameters
a=5.64, b=8.33, c=7.12 ±0.02Å
β=92.25±0.25° [ibid.]

Scattering factors
O° [3.3.1A]
Ag°, Mn° [3.3.1B]

Thermal parameters
Anisotropic, Table 4 [Boonstra, 1968]

Atomic positions
Table 3 [ibid.]

Density
(calculated) 4.507 g/cm³

Scale factor
3.101×10^4

Reference
Boonstra, E.G. (1968). The crystal structure of silver permanganate, Acta Cryst. **B24**, 1053-1062.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.41	63	0 1 1	16.38
4.50	13	-1 0 1	19.70
4.33	10	1 0 1	20.48
4.16	24	0 2 0	21.32
3.96	10	-1 1 1	22.42
3.84	10	1 1 1	23.12
3.56	31	0 0 2	25.02
3.348	79	1 2 0	26.60
3.271	50	0 1 2	27.24
3.058	100	-1 2 1	29.18
3.004	97	1 2 1	29.72
2.875	62	-1 1 2	31.08
2.819	64	2 0 0	31.72
2.786	50	1 1 2	32.10
2.670	5	2 1 0	33.54
2.586	9	0 3 1	34.66
2.531	1	-2 1 1	35.44
2.468	14	-1 2 2 +	36.38
2.334	26	2 2 0 +	38.54
2.281	32	0 1 3	39.48
2.252	2	-2 0 2	40.00
2.196	2	2 2 1	41.06
2.189	2	0 3 2	41.20
2.174	10	-2 1 2	41.50
2.168	8	2 0 2	41.62
2.156	1	1 0 3	41.86
2.098	7	2 1 2	43.08
2.087	4	1 1 3	43.32
2.082	5	0 4 0	43.42
2.057	3	-1 3 2	43.98
2.024	4	1 3 2	44.74
1.9985	21	0 4 1	45.34
1.9812	3	-2 2 2	45.76
1.9537	3	1 4 0	46.44
1.9194	7	-2 3 1	47.32
1.8908	9	-1 4 1 +	48.08
1.8769	7	1 4 1	48.46
1.8343	3	-3 0 1	49.66
1.8064	11	-2 1 3	50.48
1.8031	23	0 3 3	50.58
1.7984	14	0 4 2 +	50.72
1.7918	3	-3 1 1	50.92
1.7788	4	0 0 4	51.32
1.7490	2	-2 3 2	52.26
1.7410	11	2 1 3 +	52.52
1.7324	8	-1 3 3	52.80
1.7125	7	3 2 0	53.46
1.7084	6	2 3 2	53.60
1.7031	9	1 3 3	53.78
1.6789	14	-3 2 1 +	54.62

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.6749	11	2 4 0	54.76
1.6549	14	-3 1 2	55.48
1.6516	17	3 2 1	55.60
1.6445	10	1 1 4	55.86
1.6391	10	-2 4 1	56.06
1.6216	7	2 4 1	56.72
1.6040	9	3 1 2	57.40
1.5863	1	-1 2 4	58.10
1.5623	3	-1 5 1	59.08
1.5556	2	1 2 4 +	59.36
1.5401	12	-2 3 3	60.02
1.5313	2	-2 0 4 +	60.40
1.5087	2	0 5 2	61.40
1.5061	2	-2 1 4	61.52
1.4986	8	2 3 3	61.86
1.4780	3	2 0 4 +	62.82
1.4634	3	-1 5 2	63.52
1.4552	2	2 1 4	63.92
1.4515	5	1 5 2	64.10
1.4090	5	4 0 0	66.28
1.3927	1	-1 0 5	67.16
1.3883	1	0 6 0	67.40
1.3764	1	-3 4 1	68.06
1.3624	1	0 6 1	68.86
1.3613	1	3 4 1	68.92
1.3480	5	1 6 0	69.70
1.3393	1	-2 5 2	70.22
1.3346	1	4 2 0	70.50
1.3320	4	-1 5 3	70.66
1.3281	2	-4 0 2	70.90
1.3206	6	-1 2 5 +	71.36
1.3206	6	-3 3 3	71.36
1.3181	6	1 5 3	71.52
1.3114	1	-4 1 2	71.94
1.3048	1	2 3 4	72.36
1.3014	3	-3 1 4	72.58
1.2986	5	1 2 5	72.76
1.2928	1	4 0 2	73.14
1.2820	1	3 3 3	73.86
1.2773	1	4 1 2	74.18
1.2662	1	0 3 5	74.94
1.2565	1	1 6 2 +	75.62
1.2525	2	3 1 4	75.90
1.2450	2	-4 3 1 +	76.44
1.2336	1	-2 4 4	77.28
1.2301	2	4 3 1 +	77.54
1.2195	1	-4 1 3	78.34
1.2161	1	0 5 4	78.60

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.41	54	0 1 1	16.37
4.50	11	-1 0 1	19.69
4.34	9	1 0 1	20.47
4.17	22	0 2 0	21.32
3.96	10	-1 1 1	22.42
3.85	10	1 1 1	23.11
3.56	31	0 0 2	25.01
3.350	80	1 2 0	26.59
3.271	49	0 1 2	27.24
3.058	100	-1 2 1	29.18
3.004	98	1 2 1	29.72
2.875	64	-1 1 2	31.08
2.818	70	2 0 0	31.73
2.786	51	1 1 2	32.10
2.669	5	2 1 0	33.55
2.587	10	0 3 1	34.65
2.530	2	-2 1 1	35.45
2.469	4	2 1 1	36.36
2.468	12	-1 2 2	36.38
2.338	9	1 3 1	38.47
2.334	24	2 2 0	38.54
2.281	35	0 1 3	39.48
2.252	2	-2 0 2	40.00
2.197	2	2 2 1	41.06
2.189	1	0 3 2	41.21
2.174	10	-2 1 2	41.50
2.168	3	2 0 2	41.63
2.156	1	1 0 3	41.87
2.098	8	2 1 2	43.08
2.087	4	1 1 3	43.32
2.083	3	0 4 0	43.42
2.057	4	-1 3 2	43.98
2.024	4	1 3 2	44.74
1.9386	25	0 4 1	45.34
1.9811	3	-2 2 2	45.76
1.9534	3	1 4 0	46.45
1.9229	1	2 2 2	47.23
1.9192	8	-2 3 1	47.33
1.8921	6	2 3 1	48.05
1.8903	8	-1 4 1	48.10
1.8772	9	1 4 1	48.45
1.8342	4	-3 0 1	49.66
1.8065	10	-2 1 3	50.48
1.8033	24	0 3 3	50.57
1.7989	1	3 0 1	50.70
1.7972	2	0 4 2	50.76
1.7912	2	-3 1 1	50.94
1.7786	5	0 0 4	51.33
1.7492	2	-2 3 2	52.25
1.7410	12	2 1 3	52.52

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
1.7394	3	0	1	4	52.57
1.7326	10	-1	3	3	52.79
1.7124	9	3	2	0	53.46
1.7087	2	2	3	2	53.59
1.7028	11	1	3	3	53.79
1.6803	10	-1	1	4	54.57
1.6786	13	-3	2	1	54.63
1.6748	4	2	4	0	54.77
1.6551	16	-3	1	2	55.47
1.6516	15	3	2	1	55.60
1.6444	11	1	1	4	55.87
1.6388	11	-2	4	1	56.07
1.6216	9	2	4	1	56.71
1.6042	13	3	1	2	57.39
1.5863	1	-3	2	4	58.10
1.5625	4	-1	5	1	59.07
1.5559	1	1	2	4	59.35
1.5551	1	1	5	1	59.38
1.5399	16	-2	3	3	60.03
1.5314	2	-2	0	4	60.39
1.5304	1	-3	3	1	60.44
1.5087	2	0	5	2	61.40
1.5062	1	-2	1	4	61.51
1.4987	11	2	3	3	61.86
1.4781	3	2	0	4	62.82
1.4777	1	-3	1	3	62.84
1.4635	4	-1	5	2	63.51
1.4554	2	2	1	4	63.91
1.4514	6	1	5	2	64.11
1.4089	7	4	0	0	66.28
1.3925	1	-1	0	5	67.16
1.3883	1	0	6	0	67.40
1.3764	1	-3	4	1	68.06
1.3625	1	0	6	1	68.84
1.3613	1	3	4	1	68.92
1.3480	8	1	6	0	69.70
1.3394	1	-2	5	2	70.21
1.3346	1	4	2	0	70.50
1.3319	5	-1	5	3	70.67
1.3279	1	-4	0	2	70.91
1.3210	1	2	5	2	71.34
1.3208	4	-1	2	5	71.35
1.3208	3	-3	3	3	71.35
1.3182	6	1	5	3	71.51
1.3113	2	-4	1	2	71.95
1.3047	1	2	3	4	72.37
1.3015	4	-3	1	4	72.58
1.2988	6	1	2	5	72.75
1.2925	1	4	0	2	73.15
1.2819	2	3	3	3	73.66

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
1.2774	1	4	1	2	74.17
1.2663	1	0	3	5	74.83
1.2566	1	1	6	2	75.51
1.2563	1	-3	2	4	75.53
1.2526	3	3	1	4	75.90
1.2454	1	2	6	0	76.41
1.2448	2	-4	3	1	76.46
1.2338	1	-2	4	4	77.27
1.2304	1	-2	6	1	77.52
1.2293	2	4	3	1	77.55
1.2194	2	-4	1	3	78.35
1.2159	1	0	5	4	78.62

Structure
Cubic, $P\bar{4}3n$ (218), Z=1 [Löns and Schulz, 1967]

Lattice parameters
a=8.870 ±.004 Å [ibid.]

Scattering factors
Na^{+1}, Al^{0}, Si^{0}, Cl^{-1}, O^{-1} [3.3.1A]

Thermal parameters
Isotropic [Löns and Schulz, 1967]

Density
(calculated) 2.306 g/cm^3

Scale factor
11.30 × 10^4

Additional patterns
1. PDF card 3-0338 [Dow Chemical Co., Midland, Michigan]

Reference
Löns,J. and H. Schulz (1967). Strukturverfeinerung von Sodalith, $Na_8Si_6Al_6O_{24}Cl_2$, Acta Cryst. 24, 434-436.

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
6.267	40	1 1 0	14.12
4.436	7	2 0 0	20.00
3.966	1	2 1 0	22.40
3.622	100	2 1 1	24.56
2.805	8	3 1 0	31.88
2.560	16	2 2 2	35.02
2.371	18	3 2 1	37.92
2.217	1	4 0 0	40.66
2.091	26	4 1 1 +	43.24
1.9836	4	4 2 0	45.70
1.8908	3	3 3 2	48.08
1.8104	3	4 2 2	50.36
1.7397	2	4 3 1	52.56
1.6195	2	5 2 1	56.80
1.5681	7	4 4 0	58.84
1.5213	4	5 3 0 +	60.84
1.4784	6	4 4 2 +	62.80
1.4387	6	5 3 2	64.74
1.3686	2	5 4 1	68.50
1.3373	2	6 2 2	70.34
1.3076	2	6 3 1	72.18
1.2802	2	4 4 4	73.98
1.2071	5	7 2 1 +	79.30
1.1648	1	7 3 0	82.80
1.1265	2	6 5 1 +	86.28
1.0918	1	7 4 1 +	89.74
1.0757	1	8 2 0	91.46
1.0174	1	6 6 2	98.42
.9917	2	8 4 0	101.92
.9565	1	9 2 1 +	107.28
.9052	1	8 4 4	116.62
.8457	2	9 5 2 +	131.24
.8308	1	8 7 1 +	136.00
.8235	1	8 6 4 +	138.56
.7902	1	9 6 3 +	154.22

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.272	34	1 1 0	14.11
4.435	7	2 0 0	20.00
3.967	1	2 1 0	22.39
3.621	100	2 1 1	24.56
2.805	8	3 1 0	31.88
2.561	18	2 2 2	35.01
2.371	20	3 2 1	37.92
2.217	1	4 0 0	40.65
2.091	13	3 3 0	43.24
2.091	18	4 1 1	43.24
1.9834	5	4 2 0	45.71
1.8911	3	3 3 2	48.07
1.8106	3	4 2 2	50.36
1.7395	3	4 3 1	52.57
1.6194	3	5 2 1	56.80
1.5680	10	4 4 0	58.85
1.5212	3	5 3 0	60.84
1.5212	2	4 3 3	60.84
1.4783	3	6 0 0	62.80
1.4783	6	4 4 2	62.80
1.4389	9	5 3 2	64.73
1.3687	4	5 4 1	68.50
1.3372	3	6 2 2	70.34
1.3078	4	6 3 1	72.17
1.2803	3	4 4 4	73.98
1.2070	4	7 2 1	79.31
1.2070	1	5 5 2	79.31
1.2070	3	6 3 3	79.31
1.1647	2	7 3 0	82.81

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.1265	3	6 5 1	86.28
1.1265	1	7 3 2	86.28
1.0918	1	7 4 1	89.74
1.0918	1	8 1 1	89.74
1.0756	2	8 2 0	91.47
1.0175	2	6 6 2	98.41
1.0043	1	7 5 2	100.16
.9917	4	8 4 0	101.92
.9795	1	8 3 3	103.70
.9565	1	9 2 1	107.28
.9565	1	6 5 5	107.28
.9149	1	7 6 3	114.69
.9053	2	8 4 4	116.61
.8783	1	7 7 2	122.58
.8783	1	10 1 1	122.58
.8535	1	10 2 2	128.97
.8457	3	9 5 2	131.23
.8457	1	10 3 1	131.23
.8457	1	7 6 5	131.23
.8307	1	7 7 4	136.01
.8307	1	8 7 1	136.01
.8236	2	10 4 0	138.56
.8236	3	8 6 4	138.56
.8165	2	9 6 1	141.24
.7902	1	11 2 1	154.21
.7902	2	9 6 3	154.21
.7902	1	10 5 1	154.21

Structure
Monoclinic, $P2_1/c$ (14), Z=4 [Hyman et al. 1967].

Lattice parameters
a= 6.507±0.001 Å,
b=17.797±0.002, (published value, 17.796)
c= 8.377±0.001
β=96° 34′±2′ [ibid.]

Scattering factors
B°, Na^{+}, O^{-} [3.3.1A]

Thermal parameters
Isotropic [Hyman et al., 1967]

Density
(calculated) 2.346 g/cm³

Scale factor
3.040 ×10⁴

Additional patterns
1. PDF card 16-199. [Bouaziz, 1962]

Reference

Bouaziz, R.(1962). Contribution à l'étude radiocrystallographique de quelques borates de lithium et de sodium, Bull. Soc. Chim. France 1962, 1451.

Hyman, A., A.Perloff, F.Mauer, and S.Block (1967). The crystal structure of sodium tetraborate, Acta Cryst. 22, 815-821.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
8.89	6	0 2 0	9.94
8.32	13	0 0 1	10.62
7.53	4	0 1 1	11.74
6.08	4	0 2 1	14.56
5.23	1	1 2 0	16.94
4.62	38	1 2 -1	19.18
4.37	3	1 3 0	20.30
4.25	14	1 2 1	20.86
4.16	30	0 0 2	21.34
4.05	21	0 1 2	21.92
4.00	5	1 3 -1	22.22
3.77	41	0 2 2	23.58
3.75	33	1 3 1	23.68
3.67	3	1 4 0	24.26
3.406	63	0 3 2 +	26.14
3.273	15	1 1 2 +	27.22
3.232	100	2 0 0	27.58
3.180	30	2 1 0	28.04
3.136	19	2 0 -1	28.44
3.119	9	1 2 2	28.60
3.038	78	0 4 2 +	29.38
2.974	11	1 5 -1	30.02
2.966	13	0 6 0	30.10
2.959	26	2 2 -1	30.18
2.902	12	2 0 1 +	30.78
2.864	8	2 1 1	31.20
2.795	5	0 6 1	32.00
2.773	6	2 3 -1	32.26
2.759	18	2 2 1	32.42
2.704	23	0 5 2 +	33.10
2.696	15	1 6 0	33.20
2.676	2	2 1 -2	33.46
2.648	1	0 2 3	33.82
2.633	1	1 1 -3	34.02
2.615	3	2 4 0	34.26
2.608	3	2 3 1	34.36
2.590	1	2 2 -2	34.60
2.563	2	1 5 -2	34.98
2.550	11	1 2 -3	35.16
2.529	4	1 6 1	35.46
2.426	6	1 1 3 +	37.02
2.421	5	2 0 2	37.10
2.415	5	0 6 2	37.20
2.361	11	1 2 3 +	38.08
2.354	9	0 4 3 +	38.20
2.313	10	1 6 -2 +	38.90
2.264	2	1 3 3	39.78
2.251	5	1 7 1	40.02
2.215	4	1 6 2 +	40.70
2.169	11	0 7 2	41.60

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.154	6	2 5 -2 +	41.90
2.149	5	0 8 1	42.00
2.139	14	3 1 0	42.22
2.103	1	1 8 0	42.98
2.094	12	3 2 0 +	43.16
2.081	8	0 0 4	43.46
2.075	6	2 6 1	43.58
2.066	15	0 1 4	43.78
2.036	2	1 1 -4	44.46
2.021	25	1 7 2 +	44.82
1.9994	10	2 6 -2 +	45.32
1.9828	3	2 1 3	45.72
1.9617	8	0 8 2 +	46.24
1.9466	2	2 2 3	46.62
1.9395	4	3 4 0 +	46.80
1.9240	5	0 9 1	47.20
1.9126	2	2 7 1	47.50
1.9058	9	1 8 -2 +	47.68
1.8923	5	2 5 -3 +	48.04
1.8747	6	1 2 4 +	48.52
1.8532	9	2 7 -2 +	49.12
1.8497	10	1 8 2 +	49.22
1.8448	5	3 5 0	49.36
1.8385	18	2 1 -4 +	49.54
1.8329	13	3 4 -2 +	49.70
1.8267	6	1 3 4	49.88
1.8206	4	3 1 2	50.06
1.8098	1	2 2 -4	50.38
1.7958	3	0 5 4	50.80
1.7925	7	3 2 2	50.90
1.7641	5	2 3 -4 +	51.78
1.7609	6	1 4 4	51.88
1.7534	6	2 7 2	52.12
1.7496	9	3 5 -2 +	52.24
1.7354	2	0 8 3	52.70
1.7161	2	1 10 0	53.34
1.7031	2	0 6 4	53.78
1.6869	3	2 9 0 +	54.34
1.6727	2	2 9 -1	54.84
1.6637	6	3 6 -2 +	55.16
1.6593	4	2 1 4	55.32
1.6440	1	3 7 0	55.88
1.6364	1	2 2 4	56.16
1.6216	3	4 0 -1	56.72
1.6148	1	4 1 -1	56.98
1.6102	2	0 7 4	57.16
1.5964	3	2 9 -2 +	57.70
1.5878	2	1 9 -3 +	58.04
1.5838	2	3 1 -4	58.20
1.5764	1	3 7 -2	58.50

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
8.90	5	0 2 0	9.93
8.32	10	0 0 1	10.62
7.54	3	0 1 1	11.73
6.08	3	0 2 1	14.56
5.23	1	1 2 0	16.94
4.63	34	1 2 -1	19.17
4.37	2	1 3 0	20.30
4.25	12	1 2 1	20.86
4.16	28	0 0 2	21.34
4.05	19	0 1 2	21.92
4.00	4	1 3 -1	22.21
3.77	38	0 2 2	23.58
3.75	23	1 3 1	23.69
3.67	3	1 4 0	24.26
3.414	12	1 2 -2	26.08
3.407	54	0 3 2	26.14
3.277	2	1 4 1	27.19
3.273	9	1 1 2	27.22
3.273	3	0 5 1	27.23
3.232	100	2 0 0	27.57
3.180	29	2 1 0	28.03
3.136	18	2 0 -1	28.43
3.119	6	1 2 2	28.60
3.039	45	0 4 2	29.36
3.038	39	2 2 0	29.38
2.974	9	1 5 -1	30.02
2.966	3	0 6 0	30.10
2.958	25	2 2 -1	30.19
2.904	3	1 3 2	30.77
2.903	9	2 0 1	30.77
2.865	8	2 1 1	31.19
2.794	5	0 6 1	32.01
2.773	5	2 3 -1	32.26
2.760	18	2 2 1	32.41
2.707	1	2 0 -2	33.06
2.705	25	0 5 2	33.09
2.696	1	1 6 0	33.20
2.676	1	2 1 -2	33.46
2.648	1	0 2 3	33.82
2.633	1	1 1 -3	34.03
2.615	3	2 4 0	34.26
2.607	1	2 3 1	34.36
2.590	1	2 2 -2	34.61
2.564	1	1 5 -2	34.97
2.550	11	1 2 -3	35.16
2.530	4	1 6 1	35.46
2.431	2	0 7 1	36.94
2.431	1	2 4 1	36.94
2.427	4	1 1 3	37.01
2.422	1	2 0 2	37.09

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.415	4	0 6 2	37.19
2.366	2	1 7 0	38.00
2.362	11	1 2 3	38.07
2.354	3	0 4 3	38.20
2.353	3	2 5 -1	38.21
2.313	7	1 6 -2	38.90
2.313	5	2 4 -2	38.91
2.301	1	1 7 -1	39.11
2.264	2	1 3 3	39.78
2.251	6	1 7 1	40.02
2.218	1	2 1 -3	40.65
2.215	5	1 6 2	40.70
2.169	12	0 7 2	41.59
2.155	3	2 6 -1	41.88
2.155	4	2 5 -2	41.89
2.149	1	0 8 1	42.01
2.139	16	3 1 0	42.21
2.127	1	2 4 2	42.46
2.104	1	1 8 0	42.96
2.094	12	3 2 0	43.16
2.092	6	2 3 -3	43.22
2.087	1	3 2 -1	43.33
2.081	8	0 0 4	43.46
2.075	1	2 6 1	43.59
2.066	17	0 1 4	43.77
2.037	1	1 1 -4	44.45
2.026	1	0 6 3	44.69
2.022	4	1 8 1	44.79
2.021	25	1 7 2	44.81
2.018	1	1 5 3	44.88
2.017	1	3 1 1	44.89
2.002	4	2 5 2	45.25
1.9995	8	2 6 -2	45.32
1.9973	1	2 4 -3	45.37
1.9969	1	3 1 -2	45.38
1.9829	4	2 1 3	45.72
1.9633	2	0 3 4	46.20
1.9618	8	0 8 2	46.24
1.9602	1	3 2 -2	46.28
1.9469	2	2 2 3	46.61
1.9393	4	3 4 0	46.81
1.9376	1	1 3 -4	46.85
1.9239	5	0 9 1	47.20
1.9126	2	2 7 1	47.50
1.9065	2	1 1 4	47.66
1.9061	8	1 8 -2	47.67
1.9033	2	3 3 -2	47.74
1.8929	5	2 5 -3	48.02
1.8909	3	1 9 0	48.08
1.8760	1	2 6 2	48.49

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.8745	7	1 2 4	48.53
1.8574	1	1 9 -1	49.00
1.8532	9	2 7 -2	49.12
1.8498	7	1 8 2	49.22
1.8483	2	2 0 -4	49.26
1.8433	1	3 5 0	49.40
1.8386	2	1 7 -3	49.54
1.8384	18	2 1 -4	49.54
1.8325	4	2 8 0	49.71
1.8314	6	3 4 -2	49.74
1.8246	2	1 3 4	49.94
1.8203	3	3 1 2	50.07
1.8096	1	2 2 -4	50.38
1.7962	3	0 5 4	50.79
1.7924	7	3 2 2	50.90
1.7646	3	2 3 -4	51.76
1.7641	1	1 7 3	51.78
1.7610	5	1 4 4	51.88
1.7536	5	2 7 2	52.11
1.7499	7	3 5 -2	52.23
1.7486	1	3 3 2	52.27
1.7355	2	0 8 3	52.70
1.7159	2	1 10 0	53.35
1.7033	2	0 6 4	53.77
1.6882	1	1 5 4	54.30
1.6868	3	2 9 0	54.34
1.6727	2	2 9 -1	54.84
1.6649	2	2 0 4	55.12
1.6637	6	3 6 -2	55.16
1.6577	1	2 1 4	55.38
1.6438	1	3 7 0	55.89
1.6365	1	2 2 4	56.16
1.6215	3	4 0 -1	56.72
1.6148	1	4 1 -1	56.98
1.6101	2	0 7 4	57.16
1.5968	2	2 9 -2	57.68
1.5952	2	4 2 -1	57.74
1.5882	1	0 11 1	58.03
1.5874	1	1 9 -3	58.06
1.5840	1	3 1 -4	58.19
1.5766	1	3 7 -2	58.50
1.5695	2	1 11 0	58.78
1.5641	1	4 3 -1	59.00
1.5590	1	2 10 0	59.22
1.5574	4	3 6 2	59.29
1.5535	1	4 0 1	59.45
1.5477	3	4 1 1	59.70
1.5307	1	2 2 -5	60.43
1.5304	1	4 2 1	60.44
1.5195	1	0 8 4	60.92

Structure
Triclinic, $P\bar{1}$ (2), Z=2 [Jost and Hilmer, 1966]

Lattice parameters
a=7.96, b=9.61, c=6.67 Å
α=70.1°, β=104.3°, γ=122.5° [ibid.]

Scattering factors
Na^{+1}, Si^{0}, O^{-1} [3.3.1A]

Thermal parameters
Isotropic [Jost and Hilmer, 1966]

Density
(calculated) 1.747 g/cm³

Scale factor
0.3695×10^4

Additional patterns

1. PDF card 2-0465 [Michigan Alkali Co., Wyandotte, Michigan]
2. PDF card 3-0432 [Dow Chemical Co., Midland, Michigan]
3. PDF card 19-1241 [Jamieson and Dent Glasser, 1966]

Reference

Jamieson,P.B. and L.S. Dent Glasser (1966) Sodium silicate hydrates. I. Crystallographic data, Acta Cryst. 20, 373-376.

Jost,K.-H. and W. Hilmer(1966). Die Struktur von $Na_2H_2SiO_4 \cdot 4H_2O$, Acta Cryst. 21, 583-589.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
7.64	2	0	1	0		11.26
7.13	16	-1	1	0		12.40
6.69	39	1	0	0		13.22
6.25	100	0	0	1		14.16
5.68	41	-1	1	1		15.60
5.63	25	0	1	1		15.72
4.76	4	-1	0	1		18.62
4.49	20	-1	2	0		19.74
4.45	17	-1	2	1		19.94
4.17	20	1	1	0		21.30
4.10	53	1	-1	1		21.66
3.92	39	0	2	0		22.68
3.84	14	-2	1	0		23.12
3.78	29	0	2	1		23.52
3.63	20	-2	2	1		24.48
3.35	63	2	0	0	+	26.62
3.27	56	-1	1	2		27.26
3.17	63	1	-2	1		28.16
3.12	3	-1	3	1		28.56
3.12	3	-1	2	2	+	28.56
3.05	5	-2	0	1		29.22
3.03	30	-2	3	1		29.44
2.990	26	0	-2	1	+	29.80
2.855	9	2	0	1	+	31.30
2.840	13	-2	2	2		31.48
2.817	32	0	2	2	+	31.74
2.746	30	2	-2	1		32.58
2.731	54	1	2	1	+	32.76
2.679	4	0	-1	2		33.42
2.664	19	0	3	1		33.62
2.639	10	2	1	0		33.94
2.621	7	-3	2	1		34.16
2.609	9	1	1	2	+	34.34
2.577	2	1	-1	2		34.78
2.563	1	-3	2	0		34.98
2.502	2	-3	3	1		35.86
2.469	24	-3	1	1		36.36
2.452	1	2	1	1		36.62
2.407	6	1	-3	1		37.32
2.405	6	-1	-1	2		37.36
2.316	3	2	-3	1		38.86
2.294	9	-3	2	2		39.24
2.272	3	-3	3	2		39.64
2.230	12	1	-2	2		40.42
2.225	11	-2	4	2		40.50
2.202	11	-3	4	1	+	40.96
2.197	15	2	0	2	+	41.04
2.181	6	3	-2	1		41.36
2.156	7	-3	0	1		41.86
2.138	12	-3	1	2		42.24

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.115	3	-2 2 3 +	42.72
2.084	7	2 2 0 +	43.36
2.071	2	0 2 3	43.66
2.055	3	-1 3 3 +	44.08
2.052	6	2 -2 2	44.10
2.037	6	-1 0 3 +	44.44
2.020	14	3 -3 1 +	44.84
1.9952	1	-2 -1 2	45.42
1.9601	9	0 4 0	46.28
1.9553	7	-1 -2 2	46.40
1.9306	3	1 1 3 +	47.04
1.9225	2	-4 2 0	47.24
1.9141	5	2 -4 1	47.46
1.9095	7	3 1 0 +	47.58
1.8975	18	0 -1 3 +	47.90
1.8931	13	-3 3 3	48.02
1.8879	11	-2 4 3 +	48.16
1.8798	9	-4 4 1 +	48.38
1.8718	10	-4 3 2 +	48.60
1.8463	5	1 -1 3	49.28
1.8364	1	-2 0 3	49.60
1.8288	2	-3 5 2	49.82
1.8226	19	-1 4 3 +	50.00
1.8053	24	-2 5 0 +	50.50
1.7932	3	0 -3 2	50.86
1.7564	3	-3 5 0	51.96
1.7502	3	3 0 2	52.22
1.7295	4	-1 5 0	52.90
1.7076	5	2 0 3	53.62
1.6984	2	1 4 1	53.94
1.6944	5	-4 1 2	54.08
1.6857	3	2 3 1 +	54.38
1.6710	5	-2 5 3 +	54.90
1.6665	3	-1 2 4	55.06
1.6567	2	-3 5 3	55.34
1.6560	3	3 -3 2	55.44
1.6499	7	-4 0 1 +	55.66
1.6391	2	-1 1 4	56.06
1.6348	7	-3 -1 2 +	56.22
1.6311	4	-2 3 4	56.36
1.6242	1	3 1 2	56.62
1.6165	4	-2 -1 3 +	56.84
1.6133	4	0 1 4 +	57.04
1.5898	3	-5 3 1	57.96
1.5863	5	-1 5 3 +	58.10
1.5838	6	4 0 1 +	58.20
1.5809	7	-3 6 2	58.32
1.5710	2	2 3 2 +	58.72
1.5618	2	-2 6 2	59.10
1.5556	1	-4 5 3	59.36

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.84	2	0 1 0	11.28
7.14	16	-1 1 0	12.39
6.69	39	1 0 0	13.22
6.25	100	0 0 1	14.16
5.68	42	-1 1 1	15.59
5.64	22	0 1 1	15.71
4.76	5	-1 0 1	18.61
4.49	22	-1 2 0	19.73
4.45	18	-1 2 1	19.93
4.17	22	1 1 0	21.30
4.10	61	1 -1 1	21.65
3.92	48	0 2 0	22.67
3.84	15	-2 1 0	23.12
3.78	35	0 2 1	23.51
3.65	1	-2 1 1	24.38
3.64	24	-2 2 1	24.47
3.61	3	1 1 1	24.63
3.35	74	2 0 0	26.62
3.34	6	-1 -1 1	26.67
3.27	70	-1 1 2	27.25
3.17	79	1 -2 1	28.15
3.12	1	-1 3 1	28.56
3.12	1	-1 2 2	28.57
3.05	5	-2 0 1	29.21
3.03	38	-2 3 1	29.43
2.997	17	2 -1 1	29.79
2.996	18	0 -2 1	29.80
2.863	2	-2 3 0	31.22
2.855	9	2 0 1	31.30
2.840	15	-2 2 2	31.47
2.824	1	1 2 0	31.65
2.818	41	0 2 2	31.73
2.746	35	2 -2 1	32.58
2.733	13	-2 1 2	32.73
2.731	57	1 2 1	32.76
2.679	4	0 -1 2	33.43
2.664	24	0 3 1	33.62
2.639	12	2 1 0	33.94
2.621	7	-3 2 1	34.18
2.613	1	0 3 0	34.29
2.611	5	-2 3 2	34.32
2.609	6	1 1 2	34.35
2.578	2	1 -1 2	34.77
2.562	1	-3 2 0	34.99
2.503	2	-3 3 1	35.85
2.469	32	-3 1 1	36.35
2.451	1	2 1 1	36.64
2.408	7	1 -3 1	37.31
2.405	5	-1 -1 2	37.37
2.316	4	2 -3 1	38.85

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.294	13	-3 2 2	39.24
2.272	3	-3 3 2	39.63
2.230	15	1 -2 2	40.41
2.225	6	-2 4 2	40.50
2.202	1	2 -1 2	40.95
2.202	10	-3 4 1	40.96
2.199	5	-1 4 0	41.01
2.197	9	2 0 2	41.05
2.197	3	-1 1 3	41.06
2.188	1	0 -2 2	41.23
2.181	7	3 -2 1	41.36
2.157	9	-3 0 1	41.85
2.138	16	-3 1 2	42.24
2.115	3	-2 2 3	42.71
2.113	2	1 3 1	42.77
2.105	1	1 3 0	42.93
2.085	3	-3 4 2	43.36
2.084	4	2 2 0	43.39
2.084	4	0 0 3	43.39
2.071	1	0 2 3	43.67
2.053	10	-1 3 3	44.07
2.050	2	2 -2 2	44.13
2.039	3	2 1 2	44.40
2.037	6	-1 0 3	44.44
2.026	3	-2 1 3	44.70
2.022	4	0 4 1	44.77
2.020	18	3 -3 1	44.83
1.9953	1	-2 -1 2	45.42
1.9597	13	0 4 0	46.29
1.9556	3	-1 -2 2	46.39
1.9303	4	1 1 3	47.04
1.9284	1	-2 -2 1	47.08
1.9220	2	-4 2 0	47.25
1.9146	4	2 -4 1	47.45
1.9119	3	1 3 2	47.52
1.9098	7	3 1 0	47.57
1.8976	19	0 -1 3	47.90
1.8973	5	1 -4 1	47.91
1.8948	6	-1 -3 1	47.97
1.8933	9	-3 3 3	48.01
1.8892	4	-3 0 2	48.12
1.8876	6	-2 4 3	48.17
1.8801	10	-4 4 1	48.37
1.8783	3	0 3 3	48.42
1.8718	10	-4 3 2	48.60
1.8716	2	-3 5 1	48.61
1.8485	8	1 -1 3	49.25
1.8366	1	-2 0 3	49.59
1.8294	1	-3 5 2	49.80
1.8227	11	3 1 1	50.00

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.8224	18	-1 4 3	50.01
1.8131	1	-1 5 1	50.28
1.8111	2	-3 4 3	50.34
1.8062	19	-2 5 0	50.49
1.8059	15	2 2 2	50.50
1.8058	3	3 -1 2	50.50
1.7930	3	0 -3 2	50.88
1.7586	4	-3 5 0	51.95
1.7499	4	3 0 2	52.23
1.7294	6	-1 5 0	52.90
1.7079	8	2 0 3	53.62
1.6987	3	1 4 1	53.93
1.6941	6	-4 1 2	54.09
1.6860	3	2 3 1	54.37
1.6848	1	2 -1 3	54.41
1.6722	1	0 -2 3	54.86
1.6711	4	-2 5 3	54.89
1.6697	4	-2 -2 2	54.94
1.6655	1	-1 2 4	55.10
1.6590	2	-3 5 3	55.33
1.6562	3	3 -3 2	55.43
1.6511	4	-4 3 3	55.62
1.6496	9	-4 0 1	55.67
1.6393	2	-1 1 4	56.06
1.6357	1	-4 4 3	56.19
1.6350	8	-3 -1 2	56.21
1.6349	1	-2 2 4	56.22
1.6307	1	-2 3 4	56.38
1.6244	1	3 1 2	56.61
1.6192	1	-1 3 4	56.81
1.6134	4	-2 -1 3	56.84
1.6132	4	0 1 4	57.04
1.6119	3	-4 5 0	57.09
1.5902	3	-5 3 1	57.95
1.5884	1	3 2 1	58.02
1.5875	1	4 -4 1	58.05
1.5866	2	-3 6 1	58.09
1.5861	3	-1 5 3	58.11
1.5843	3	4 0 1	58.18
1.5840	2	-2 -3 1	58.19
1.5836	2	2 -4 2	58.21
1.5808	8	-3 6 2	58.32
1.5719	1	-2 1 4	58.69
1.5710	1	2 3 2	58.72
1.5617	2	-2 6 2	59.11
1.5556	1	-4 5 3	59.36
1.5530	2	-3 -2 1	59.47
1.5498	1	-1 0 4	59.60
1.5428	5	-5 4 2	59.91
1.5424	2	-5 3 0	59.92

Structure

Tetragonal, $P4_2/nbc$ (133), Z=8 [McDonald et al., 1964]

Lattice parameters

a=9.020±0.003, c=13.686±0.003Å [ibid.]

Scattering factors

Sn° [3.3.1B];
Na°, F^{-1} [Berghuis et al., 1955]

Thermal parameters

Isotropic: Sn 1.70; F(1) 2.29; F(2)1.91; F(3) 2.71; Na(1) 1.92; Na(2) 1.97

Density

(calculated) 4.24g/cm³ [McDonald et al., 1964]

Scale factor

125.3×10^4

Additional patterns

1. PDF card 15-619[Kriegsmann and Kessler, 1962]
2. PDF card 16-796[Donaldson and O'Donoghue 1964]

Reference

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Donaldson, J.D. and J.D. O'Donaghue(1964). Complex tin fluorides, J. Chem.Soc.1964, 271-280.

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McDonald,R.R., A.C. Larson, and D.T.Cromer (1964). The crystal structure of sodium pentafluorodistannate(II), $NaSn_2F_5$, Acta Cryst. 17, 1104-1108.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(^{\circ})$ $\lambda = 1.54056$ Å
6.84	2	0 0 2	12.94
4.51	42	2 0 0	19.68
4.28	1	2 0 1	20.72
3.474	100	2 1 2	25.62
3.422	23	0 0 4	26.02
3.188	9	2 2 0	27.96
3.015	5	1 1 4 +	29.60
2.852	10	3 1 0	31.34
2.725	15	2 0 4	32.84
2.265	4	2 1 5	39.76
2.255	3	4 0 0	39.94
2.224	1	4 0 1	40.52
2.191	5	3 1 4	41.16
2.160	1	4 1 1	41.78
2.126	5	3 3 0	42.48
2.084	30	4 1 2	43.36
2.035	1	4 0 6	44.48
2.017	2	4 2 0	44.90
1.9853	17	2 1 6	45.66
1.8827	4	4 0 4	48.30
1.8058	14	3 3 4	50.50
1.7108	3	0 0 8	53.52
1.6269	4	5 2 2	56.52
1.5994	1	2 0 8	57.58
1.5785	8	4 1 6	58.40
1.5750	5	2 1 8	58.56
1.5715	3	5 1 4	58.70
1.5471	3	5 3 0	59.72
1.5074	1	2 2 8	61.46
1.5034	3	6 0 0	61.64
1.4671	2	3 1 8	63.34
1.4262	1	6 2 0	65.38
1.4094	3	5 3 4	66.26
1.3796	4	5 4 2	67.88
1.3764	4	6 0 4	68.06
1.3500	1	5 2 6	69.58
1.3327	2	3 3 8	70.62
1.3165	2	6 2 4	71.62
1.2959	2	2 1 10	72.94
1.2193	2	7 2 2	78.36
1.1986	1	5 4 6	79.96
1.1602	2	4 1 10	83.20
1.1474	1	5 3 8	84.34
1.1292	1	6 0 8	86.02
1.1041	2	7 4 2 +	88.48
1.0838	1	7 2 6	90.06
1.0045	2	7 4 6 +	100.14

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.84	1	0 0 2	12.93
4.51	40	2 0 0	19.67
4.28	1	2 0 1	20.72
3.475	100	2 1 2	25.61
3.422	22	0 0 4	26.02
3.189	9	2 2 0	27.95
3.022	1	2 1 3	29.53
3.015	5	1 1 4	29.60
2.852	10	3 1 0	31.33
2.726	18	2 0 4	32.83
2.265	5	2 1 5	39.76
2.255	2	4 0 0	39.95
2.225	2	4 0 1	40.51
2.191	6	3 1 4	41.17
2.160	1	4 1 1	41.78
2.126	6	3 3 0	42.48
2.084	37	4 1 2	43.39
2.035	1	2 0 6	44.47
2.017	3	4 2 0	44.90
1.9855	21	2 1 6	45.65
1.8828	5	4 0 4	48.30
1.8058	17	3 3 4	50.50
1.7107	4	0 0 8	53.52
1.6269	6	5 2 2	56.52
1.5995	2	2 0 8	57.58
1.5789	11	4 1 6	58.40
1.5750	1	2 1 8	58.56
1.5714	3	5 1 4	58.71
1.5469	4	5 3 0	59.73
1.5075	1	2 2 8	61.45
1.5033	4	6 0 0	61.65
1.4671	3	3 1 8	63.34
1.4492	1	6 1 2	64.21
1.4262	1	6 2 0	65.38
1.4095	4	5 3 4	66.25
1.3798	5	5 4 2	67.87
1.3763	3	6 0 4	68.06
1.3501	2	5 2 6	69.58
1.3328	3	3 3 8	70.61
1.3164	2	6 2 4	71.63
1.2960	3	2 1 10	72.83
1.2192	3	7 2 2	78.37
1.1985	2	5 4 6	79.98
1.1748	1	6 4 4	81.94
1.1603	3	4 1 10	83.19
1.1474	2	5 3 8	84.34
1.1293	2	6 0 8	86.02
1.1041	1	8 1 2	88.47
1.1041	2	7 4 2	88.47
1.0887	2	7 2 6	90.06

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.0708	1	8 0 4	92.00
1.0598	1	5 2 10	93.24
1.0050	1	3 3 12	100.07
1.0045	2	7 4 6	100.14
1.0045	1	8 1 6	100.14

Structure

Monoclinic, $P2_1$ (4), Z=2, [Okaya and Stemple, 1966]

Lattice parameters

a=7.715±0.003, b=6.004±0.003, c=6.231±0.003Å, β=100.1±0.1° [ibid.]

Scattering factors

H^0, C^0, O^0 [3.3.1A]

Thermal parameters

Anisotropic for oxygen and carbon, isotropic for hydrogen, Table 1(b)[Okaya and Stemple, 1966]

Atomic positions

Table 1(a)[ibid.]

Density

(calculated) 1.754 g/cm³

Scale factor

0.4175 × 10^4

Additional patterns

1. PDF card 4-0333 [Inst. Phys. Univ. College, Cardiff, Wales]. This card may represent a different polymorph.

Reference

Okaya,H. and N.R. Stemple (1966). Refinement of the structure of d-tartaric acid by x-ray and neutron diffraction, Acta Cryst. 21, 237-243.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.60	13	1 0 0	11.64
5.24	7	-1 0 1	16.90
4.71	20	1 1 0	18.82
4.41	18	1 0 1	20.12
4.29	100	0 1 1	20.68
3.95	18	-1 1 1	22.50
3.80	4	2 0 0	23.40
3.55	26	1 1 1	25.04
3.209	5	2 1 0	27.78
3.066	15	0 0 2	29.10
3.033	5	-2 1 1 +	29.42
3.002	36	0 2 0 +	29.74
2.791	24	1 2 0	32.04

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.731	2	0 1 2	32.76
2.709	1	-1 1 2	33.04
2.696	1	0 2 1	33.20
2.685	7	1 0 2 +	33.34
2.605	2	-1 2 1	34.40
2.532	8	3 0 0	35.42
2.499	24	-3 0 1	35.90
2.482	11	1 2 1	36.16
2.451	21	1 1 2	36.64
2.403	17	-2 1 2	37.40
2.355	1	2 2 0	38.18
2.333	2	3 1 0	38.56
2.308	7	-3 1 1	39.00
2.283	1	-2 2 1	39.44
2.146	1	-3 0 2	42.08
2.122	4	2 2 1	42.56
2.068	2	-1 0 3 +	43.74
2.021	3	-3 1 2	44.82
1.9746	2	-2 2 2	45.92
1.9490	2	-2 0 3	46.56
1.9356	5	3 2 0 +	46.90
1.9209	5	-3 2 1	47.28
1.9028	3	0 3 1	47.76
1.8696	1	-1 3 1	48.66
1.8532	3	-2 1 3	49.12
1.8213	2	-4 1 1 +	50.04
1.8058	1	1 1 3	50.50
1.7769	1	2 2 2	51.38
1.7705	2	2 3 0	51.58
1.7584	1	-4 0 2	51.96
1.7269	1	3 1 2	52.98
1.6897	1	0 2 3	54.24
1.6626	4	4 1 1	55.20
1.6045	1	4 2 0	57.38
1.6009	1	1 2 3	57.52
1.5908	1	-2 3 2	57.92
1.5701	1	3 3 0	58.76
1.5623	1	-3 3 1 +	59.08
1.5457	1	3 2 2	59.78
1.5336	1	0 0 4	60.30
1.5008	1	0 4 0	61.76
1.4827	1	3 3 1	62.60
1.4725	1	1 4 0	63.08
1.3821	1	-1 2 4	67.74
1.3803	1	-2 4 1	67.84
1.3102	1	2 1 4	72.02
1.3048	1	-5 1 3	72.36
1.2874	1	2 3 3	73.50
1.2853	1	-6 0 1	73.64

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
7.60	11	1	0	0	11.64
5.24	6	-1	0	1	16.90
4.71	20	1	1	0	18.82
4.41	17	1	0	1	20.12
4.29	100	0	1	1	20.68
3.95	18	-1	1	1	22.50
3.80	4	2	0	0	23.40
3.55	27	1	1	1	25.04
3.210	6	2	1	0	27.77
3.067	17	0	0	2	29.09
3.035	1	-1	0	2	29.41
3.035	4	-2	1	1	29.41
3.002	35	0	2	0	29.74
3.002	4	2	0	1	29.74
2.792	28	1	2	0	32.03
2.731	3	0	1	2	32.76
2.709	1	-1	1	2	33.05
2.696	1	0	2	1	33.20
2.685	5	1	0	2	33.34
2.685	2	2	1	1	33.34
2.605	2	-1	2	1	34.40
2.532	9	3	0	0	35.42
2.500	29	-3	0	1	35.89
2.481	12	1	2	1	36.17
2.451	26	1	1	2	36.53
2.402	20	-2	1	2	37.40
2.355	1	2	2	0	38.18
2.333	2	3	1	0	38.56
2.308	8	-3	1	1	38.99
2.283	1	-2	2	1	39.43
2.146	1	-3	0	2	42.07
2.123	6	2	2	1	42.55
2.070	1	2	1	2	43.70
2.058	2	-1	0	3	43.75
2.021	4	-3	1	2	44.81
1.9746	2	-2	2	2	45.92
1.9487	2	-2	0	3	46.57
1.9356	3	0	1	3	46.90
1.9354	3	3	2	0	46.91
1.9211	6	-3	2	1	47.28
1.9025	3	0	3	1	47.76
1.8697	1	-1	3	1	48.66
1.8535	4	-2	1	3	49.11
1.8224	1	1	3	1	50.01
1.8211	2	-4	1	1	50.05
1.8053	1	1	1	3	50.51
1.7769	1	2	2	2	51.38
1.7705	3	2	3	0	51.58
1.7584	1	-4	0	2	51.96
1.7272	1	3	1	2	52.97

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.6900	1	0	2	3	54.23
1.6626	5	4	1	1	55.20
1.6345	1	-2	2	3	56.23
1.6048	1	4	2	0	57.37
1.6012	1	1	2	3	57.51
1.5907	1	-2	3	2	57.92
1.5700	1	3	3	0	58.76
1.5624	1	-3	3	1	59.08
1.5572	1	-1	0	4	59.29
1.5459	1	3	2	2	59.77
1.5335	1	0	0	4	60.30
1.5073	1	-1	1	4	61.46
1.5010	1	0	4	0	61.75
1.4828	1	3	3	1	62.60
1.4726	1	1	4	0	63.08
1.4635	1	-3	3	2	63.51
1.4209	1	1	4	1	65.65
1.3823	1	-1	2	4	67.73
1.3805	1	-2	4	1	67.83
1.3103	1	2	1	4	72.01
1.3048	1	-5	1	3	72.36
1.2874	1	2	3	3	73.50
1.2852	1	-6	0	1	73.65

Structure

Orthorhombic, $P2_12_12_1$ (19), Z=4, [Gramaccioli, 1966]

Lattice parameters

a=11.190, b=10.463, c=7.220Å [ibid.]

Scattering factors

C°, N°, H°, [3.3.1A];
Zn° [3.3.1A], corrected for the real part of the dispersion effect [3.3.2B]

Thermal parameters

Isotropic: Zn 1.93; C(1) 1.94; C(2)1.95; C(3) 2.19; C(4) 2.68; C(5) 2.35; N 2.20; O(1) 2.33; O(2) 2.25; O(3) 2.61; O(4) 2.88; O(5) 3.08; O(6) 2.86; H(1) through H(11) as given by Gramaccioli [1966].

Density

(calculated) 1.937 g/cm³ [Gramaccioli,1966]

Scale factor

3.869×10^4

Reference

Gramaccioli,C.M.(1966). The crystal structure of zinc glutamate dihydrate, Acta Cryst. 21, 600-605.

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.64	35	1 1 0	11.58
5.94	32	0 1 1	14.90
5.59	46	2 0 0	15.84
5.25	100	1 1 1 +	16.88
4.93	51	2 1 0	17.96
4.23	48	0 2 1	20.96
4.07	74	2 1 1	21.80
3.96	87	1 2 1	22.42
3.82	2	2 2 0	23.26
3.61	2	0 0 2	24.64
3.435	21	1 0 2	25.92
3.378	2	2 2 1	26.36
3.329	4	1 3 0	26.76
3.314	16	3 0 1	26.88
3.264	7	1 1 2	27.30
3.160	6	3 1 1	28.22
3.140	7	0 3 1	28.40
3.038	18	3 2 0	29.38
3.023	23	1 3 1	29.52
2.970	10	0 2 2	30.06
2.963	7	2 3 0	30.14
2.914	1	2 1 2	30.66
2.872	12	1 2 2	31.12
2.798	4	4 0 0 +	31.96
2.738	2	2 3 1	32.68
2.703	8	4 1 0	33.12
2.624	4	2 2 2	34.14
2.617	4	0 4 0	34.24
2.608	9	4 0 1	34.36
2.595	7	3 0 2	34.54
2.517	6	3 1 2	35.64
2.509	10	0 3 2	35.76
2.466	1	4 2 0	36.40
2.460	3	0 4 1	36.50
2.448	1	1 3 2	36.68
2.403	15	1 4 1 +	37.40
2.370	1	2 4 0	37.94
2.346	3	0 1 3	38.34
2.334	3	4 2 1	38.54
2.324	11	3 2 2	38.72
2.295	17	1 1 3	39.22
2.290	22	2 3 2	39.32
2.251	6	2 4 1	40.02
2.211	2	2 0 3	40.78
2.163	8	4 1 2 +	41.72
2.146	9	1 2 3	42.08
2.138	8	5 0 1	42.24
2.118	2	0 4 2	42.66
2.094	6	5 1 1	43.16
2.083	5	4 3 1	43.28

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
2.081	7	1 4 2 +	43.44
2.057	8	1 5 0 +	43.98
2.053	7	3 4 1	44.08
2.037	8	4 2 2 +	44.44
2.022	2	3 0 3	44.78
2.009	3	0 5 1	45.08
1.9853	4	3 1 3	45.66
1.9803	7	2 4 2 +	45.78
1.9020	1	5 0 2	47.78
1.8916	5	4 5 1	48.06
1.8864	6	3 2 3	48.20
1.8711	10	5 1 2	48.62
1.8668	7	4 3 2 +	48.74
1.8469	1	4 4 1	49.30
1.8420	2	3 4 2	49.44
1.8364	6	6 1 0	49.60
1.8233	7	5 3 1 +	49.98
1.8104	5	0 5 2	50.36
1.8058	4	6 0 1 +	50.50
1.7971	2	4 1 3	50.76
1.7873	3	1 5 2	51.06
1.7795	3	6 1 1	51.30
1.7692	3	3 5 1 +	51.62
1.7565	1	1 1 4	52.02
1.7496	3	3 3 3 +	52.24
1.7440	2	0 6 0	52.42
1.7227	3	2 5 2 +	53.12
1.7179	3	2 0 4	53.28
1.7066	2	0 2 4 +	53.66
1.7008	2	5 4 0	53.86
1.6949	2	2 1 4	54.06
1.6886	4	4 4 2 +	54.26
1.6760	2	1 6 1 +	54.72
1.6648	2	2 6 0	55.12
1.6391	2	5 0 3	56.06
1.6322	4	2 2 4 +	56.32
1.6285	3	3 5 2	56.46
1.6164	2	4 3 3	56.92
1.6035	2	6 3 1	57.42
1.5999	3	3 4 3	57.56
1.5868	5	1 3 4	58.08
1.5794	3	6 2 2	58.38
1.5638	2	5 2 3 +	59.02
1.5604	2	7 0 1	59.16
1.5552	2	1 6 2	59.36
1.5514	2	3 2 4	59.54
1.5434	1	3 6 1	59.88
1.5286	1	5 5 0	60.52
1.5119	1	2 6 2	61.26
1.5006	2	4 1 4	61.76

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
7.64	31	1 1 0	11.57
5.94	32	0 1 1	14.90
5.59	50	2 0 0	15.83
5.25	100	1 1 1	16.88
5.23	22	0 2 0	16.93
4.93	56	2 1 0	17.96
4.24	54	0 2 1	20.95
4.07	34	2 1 1	21.80
3.96	100	1 2 1	22.42
3.82	2	2 2 0	23.26
3.61	2	0 0 2	24.64
3.436	25	1 0 2	25.91
3.377	3	2 2 1	26.37
3.330	3	1 3 0	26.75
3.314	18	3 0 1	26.88
3.264	8	1 1 2	27.30
3.159	7	3 1 1	28.24
3.140	8	0 3 1	28.40
3.037	21	3 2 0	29.38
3.024	25	1 3 1	29.52
2.971	12	0 2 2	30.05
2.960	4	2 3 0	30.17
2.913	1	2 1 2	30.66
2.872	15	1 2 2	31.12
2.799	2	3 2 1	31.94
2.797	3	4 0 0	31.97
2.733	2	2 3 1	32.67
2.703	10	4 1 0	33.12
2.624	5	2 2 2	34.14
2.616	1	0 4 0	34.25
2.609	11	4 0 1	34.35
2.594	8	3 0 2	34.55
2.518	7	3 1 2	35.63
2.508	12	0 3 2	35.77
2.467	1	4 2 0	36.39
2.459	4	0 4 1	36.51
2.446	1	1 3 2	36.69
2.402	4	3 3 1	37.40
2.402	16	1 4 1	37.41
2.370	1	2 4 0	37.94
2.345	4	0 1 3	38.35
2.334	3	4 2 1	38.53
2.324	15	3 2 2	38.71
2.296	21	1 1 3	39.21
2.289	20	2 3 2	39.33
2.251	8	2 4 1	40.01
2.211	3	2 0 3	40.78
2.163	6	4 1 2	41.71
2.163	5	2 1 3	41.72
2.146	12	1 2 3	42.07

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
2.138	8	5	0	1	42.24
2.118	2	0	4	2	42.65
2.094	8	5	1	1	43.16
2.089	2	4	3	1	43.28
2.081	2	3	3	2	43.44
2.081	8	1	4	2	43.45
2.058	2	5	2	0	43.97
2.057	8	1	5	0	43.98
2.053	5	3	4	1	44.07
2.037	10	4	2	2	44.44
2.036	1	2	2	3	44.45
2.022	2	3	0	3	44.78
2.010	5	0	5	1	45.07
1.9855	5	3	1	3	45.65
1.9809	5	2	4	2	45.77
1.9808	1	0	3	3	45.77
1.9788	2	5	2	1	45.82
1.9782	3	1	5	1	45.83
1.9021	2	5	0	2	47.78
1.8915	6	2	5	1	48.06
1.8862	5	3	2	3	48.20
1.8715	15	5	1	2	48.61
1.8675	2	4	3	2	48.72
1.8673	1	1	3	3	48.73
1.8471	1	4	4	1	49.29
1.8419	2	3	4	2	49.44
1.8361	8	6	1	0	49.61
1.8250	2	3	5	0	49.93
1.8244	6	4	0	3	49.95
1.8226	6	5	3	1	50.00
1.8104	7	0	5	2	50.36
1.8057	1	6	0	1	50.50
1.8050	1	0	0	4	50.52
1.7973	2	4	1	3	50.75
1.7872	4	1	5	2	51.06
1.7794	3	6	1	1	51.30
1.7711	1	0	4	3	51.56
1.7594	4	3	5	1	51.61
1.7567	1	1	1	4	52.01
1.7494	2	3	3	3	52.25
1.7493	2	1	4	3	52.25
1.7438	2	0	6	0	52.43
1.7227	1	4	2	3	53.12
1.7225	4	2	5	2	53.13
1.7178	2	2	0	4	53.28
1.7069	1	6	2	1	53.65
1.7063	2	0	2	4	53.67
1.7005	2	5	4	0	53.87
1.6951	2	2	1	4	54.05
1.6887	4	4	4	2	54.28

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
1.6885	2	2	4	3	54.28
1.6868	1	1	2	4	54.34
1.6760	2	1	6	1	54.72
1.6757	1	4	5	0	54.73
1.6648	3	2	6	0	55.12
1.6389	2	5	0	3	56.07
1.6323	2	4	5	1	56.32
1.6321	4	2	2	4	56.32
1.6287	1	3	5	2	56.45
1.6166	3	4	3	3	56.91
1.6035	3	6	3	1	57.42
1.5993	3	3	4	3	57.56
1.5868	8	1	3	4	58.06
1.5796	4	6	2	2	58.37
1.5639	1	5	2	3	59.01
1.5636	1	1	5	3	59.03
1.5608	3	7	0	1	59.15
1.5550	3	1	6	2	59.39
1.5516	2	3	2	4	59.53
1.5432	2	3	6	1	59.89
1.5285	1	5	5	0	60.52
1.5118	1	2	6	2	61.26
1.5010	3	4	1	4	61.75
1.4956	1	7	2	1	62.00
1.4954	2	5	5	1	62.01
1.4833	1	5	3	3	62.57
1.4799	1	4	6	0	62.73
1.4726	3	3	3	4	63.07
1.4542	2	3	5	3	63.97
1.4513	3	1	7	1	64.11
1.4497	1	4	6	1	64.19
1.4476	2	7	1	2	64.30
1.4472	1	3	6	2	64.31
1.4304	1	0	1	5	65.16
1.4246	1	7	3	1	65.46
1.4189	1	5	2	3	65.76
1.4160	1	2	7	1	65.91
1.4075	2	5	5	2	66.36
1.3997	4	6	4	2	66.76
1.3864	1	8	1	0	67.50
1.3802	2	3	4	4	67.85
1.3692	1	2	6	3	68.47
1.3671	1	6	5	1	68.59
1.3543	2	7	4	0	68.76
1.3573	1	6	3	3	69.12
1.3569	1	5	2	4	69.18
1.3512	2	5	6	1	69.51
1.3508	2	2	2	5	69.54
1.3356	1	3	1	5	70.44
1.3316	1	7	0	3	70.69

Zinc Molybdate, $Zn_2Mo_3O_8$ (hexagonal)

Structure
Hexagonal, $P6_3mc$ (186), Z=2 [Ansell and Katz,1966]

Lattice parameters
a=5.759±0.004, c=9.903±0.005Å [ibid.]

Scattering factors
O^{-1} [3.3.1A]; Zn^{+2} and Mo^{+4} [Thomas and Umeda 1957], corrected for the real part of the anomalous dispersion [Dauben and Templeton,1955]

Thermal parameters
Isotropic [Ansell and Katz,1966]

Density
(calculated) 6.381 g/cm³

Scale factor
4.920×10^4

Additional patterns

1. PDF card 16-663 [Donohue and Katz,1964]

Reference

Ansell,G.B. and L. Katz (1966). A refinement of the crystal structure of zinc molybdenum(IV) oxide, $Zn_2Mo_3O_8$, Acta Cryst. **21**, 482-485.

Dauben, C.H. and D.H. Templeton (1955). A table of dispersion corrections for x-ray scattering of atoms, Acta Cryst. **8**, 841-842.

Donohue, P.C. and L. Katz (1964). A lithium-scandium-molybdenum(IV) oxide, Nature **201**, 180-181.

Thomas, L. H. and K. Umeda (1957). Atomic scattering factors calculated from the TFD atomic model,J.Chem.Phys.26,293-303.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.95	78	0 0 2	17.90
4.45	18	1 0 1	19.92
3.51	100	1 0 2	25.32
2.879	3	1 1 0	31.04
2.753	37	1 0 3	32.50
2.489	85	1 1 2	36.06
2.475	24	0 0 4	36.26
2.419	75	2 0 1	37.14
2.228	16	2 0 2	40.46
2.220	10	1 0 4	40.60
1.9894	39	2 0 3	45.56
1.8849	7	2 1 0	48.24
1.8776	3	1 1 4	48.44
1.8518	12	2 1 1	49.16
1.8406	2	1 0 5	49.48
1.7571	21	2 0 4	52.00
1.6505	4	0 0 6	55.64
1.6370	33	2 1 3	56.14
1.5759	17	3 0 2	58.52
1.5672	5	1 0 6	58.88
1.5509	41	2 0 5	59.56
1.4999	3	2 1 4	61.80
1.4848	5	3 0 3	62.50
1.4399	23	2 2 0	64.68
1.4320	3	1 1 6	65.08
1.3825	5	2 2 2	67.72
1.3793	3	3 0 4	67.90
1.3764	5	2 0 6	68.06
1.3655	3	2 1 5	68.68
1.3610	4	1 0 7	68.94
1.3323	4	3 1 2	70.64
1.2758	2	3 1 3	74.28
1.2732	3	3 0 5	74.46
1.2467	2	4 0 0	76.32
1.2445	7	2 2 4	76.48
1.2371	5	4 0 1 +	77.02
1.2304	4	2 0 7	77.52
1.2092	1	4 0 2	79.14
1.2013	1	1 0 8	79.76
1.1713	2	3 0 6	82.24
1.1664	3	4 0 3	82.66
1.1441	2	3 2 0	84.64
1.1371	1	1 1 8	85.28
1.1341	2	3 1 5	85.56
1.1316	7	2 1 7	85.80
1.1147	10	3 2 2 +	87.42
1.1089	1	2 0 8	88.00
1.0850	3	2 2 6	90.46
1.0820	3	4 1 1 +	90.78
1.0774	2	3 0 7	91.28

Calculated Pattern *(Peak heights)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.0746	1	1 0 9	91.58
1.0630	4	4 1 2	92.88
1.0603	3	3 1 6	93.18
1.0551	6	4 0 5	93.78
1.0386	4	3 2 4	95.74
1.0336	2	4 1 3	96.36
1.0067	4	2 0 9	99.84
.9975	1	5 0 0	101.10
.9950	1	4 0 6	101.46
.9926	3	5 0 1 +	101.80
.9903	3	0 0 10 +	102.12
.9891	2	3 1 7	102.30
.9548	4	5 0 3	107.56
.9539	2	4 1 5	107.70
.9503	2	2 1 9	108.30
.9424	1	4 2 0	109.64
.9403	6	3 2 6	110.00
.9385	7	2 2 8 +	110.32
.9361	4	4 0 7 +	110.74
.9252	1	5 0 4	112.72
.9228	1	3 1 8	113.18
.9203	1	2 0 10	113.64
.9176	1	3 0 9	114.16
.9063	2	4 2 3	116.40
.8909	2	5 0 5	119.68
.8896	1	3 2 7	119.96
.8809	1	4 2 4	121.96
.8785	1	4 0 8	122.52
.8645	1	5 1 3	126.00
.8626	2	4 1 7	126.50
.8611	1	3 1 9	126.90
.8511	7	4 2 5 +	129.66
.8468	3	2 0 11	130.92
.8423	1	5 1 4	132.26
.8403	5	3 2 8	132.90
.8312	2	6 0 0	135.84
.8250	2	4 0 9 +	138.02
.8199	2	4 3 0	139.92
.8185	1	4 2 6	140.48
.8171	3	4 3 1 +	141.00
.8159	5	2 2 10 +	141.50
.8152	5	5 0 7	141.78
.8139	3	1 0 12	142.30
.8124	3	2 1 11	142.94
.7960	8	5 2 1 +	150.80
.7916	1	3 0 11	153.32
.7884	5	6 0 4 +	155.38
.7873	1	5 1 6	156.12
.7844	1	4 2 7	158.24
.7835	1	2 0 12	158.94

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.99	4	1 0 0	17.77
4.95	68	0 0 2	17.90
4.45	17	1 0 1	19.92
3.51	100	1 0 2	25.33
2.880	3	1 1 0	31.03
2.753	39	1 0 3	32.50
2.494	27	2 0 0	35.98
2.489	78	1 1 2	36.05
2.476	19	0 0 4	36.25
2.418	86	2 0 1	37.15
2.227	19	2 0 2	40.47
2.218	5	1 0 4	40.65
1.9898	47	2 0 3	45.55
1.8851	8	2 1 0	48.24
1.8773	2	1 1 4	48.45
1.8518	15	2 1 1	49.16
1.8408	2	1 0 5	49.47
1.7569	27	2 0 4	52.01
1.6506	5	0 0 6	55.54
1.6395	12	3 0 1	56.04
1.6370	38	2 1 3	56.14
1.5760	22	3 0 2	58.52
1.5669	7	1 0 6	58.89
1.5509	56	2 0 5	59.56
1.4998	4	2 1 4	61.81
1.4848	7	3 0 3	62.50
1.4397	34	2 2 0	64.69
1.4319	4	1 1 6	65.08
1.3825	6	2 2 2	67.72
1.3802	1	3 0 4	67.85
1.3763	6	2 0 6	68.06
1.3655	4	2 1 5	68.68
1.3610	6	1 0 7	68.94
1.3323	6	3 1 2	70.64
1.2758	2	3 1 3	74.28
1.2734	4	3 0 5	74.45
1.2469	2	4 0 0	76.31
1.2446	10	2 2 4	76.47
1.2376	4	0 0 8	76.96
1.2371	6	4 0 1	77.02
1.2305	6	2 0 7	77.51
1.2091	1	4 0 2	79.15
1.2014	2	1 0 8	79.75
1.1713	3	3 0 6	82.24
1.1664	4	4 0 3	82.56
1.1442	3	3 2 0	84.53
1.1372	1	1 1 8	85.27
1.1341	2	3 1 5	85.57
1.1315	11	2 1 7	85.81
1.1148	18	3 2 2	87.41

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
1.1135	4	4 0 4	87.53
1.1088	2	2 0 8	88.01
1.0850	5	2 2 6	90.46
1.0818	4	4 1 1	90.80
1.0811	1	3 2 3	90.88
1.0774	3	3 0 7	91.28
1.0745	1	1 0 9	91.59
1.0630	6	4 1 2	92.88
1.0602	2	3 1 6	93.20
1.0552	10	4 0 5	93.77
1.0386	7	3 2 4	95.74
1.0336	3	4 1 3	96.36
1.0067	7	2 0 9	99.84
.9975	2	5 0 0	101.11
.9949	2	4 0 6	101.47
.9929	2	3 0 8	101.76
.9925	4	5 0 1	101.81
.9907	2	3 2 5	102.06
.9903	2	0 0 10	102.12
.9890	2	3 1 7	102.30
.9598	1	3 3 0	106.74
.9546	9	5 0 3	107.55
.9538	3	4 1 5	107.72
.9503	3	2 1 9	108.30
.9425	1	4 2 0	109.62
.9403	11	3 2 6	110.06
.9386	9	2 2 8	110.30
.9383	5	4 2 1	110.36
.9365	1	1 1 10	110.68
.9354	2	4 0 7	110.87
.9252	2	5 0 4	112.72
.9224	1	3 1 8	113.24
.9204	3	2 0 10	113.63
.9175	3	3 0 9	114.17
.9086	1	4 1 6	115.94
.9063	4	4 2 3	116.40
.8958	1	5 1 0	118.61
.8949	1	3 3 4	118.79

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
.8909	4	5 0 5	119.58
.8896	2	3 2 7	119.96
.8859	1	1 0 11	120.79
.8809	3	4 2 4	121.96
.8786	1	4 0 8	122.53
.8767	1	2 1 10	122.95
.8645	2	5 1 3	126.00
.8626	4	4 1 7	126.49
.8611	2	3 1 9	126.89
.8537	1	5 0 6	128.92
.8511	17	4 2 5	129.56
.8508	2	3 0 10	129.75
.8468	8	2 0 11	130.92
.8423	3	5 1 4	132.26
.8402	12	3 2 8	132.91
.8312	7	6 0 0	135.84
.8252	2	0 0 12	137.94
.8250	6	4 0 9	138.02
.8199	4	4 3 0	139.92
.8185	2	4 2 6	140.48
.8174	2	4 1 8	140.92
.8171	6	4 3 1	141.01
.8162	1	5 1 5	141.39
.8159	14	2 2 10	141.49
.8152	12	5 0 7	141.77
.8142	2	1 0 12	142.20
.8124	9	2 1 11	142.95
.8089	2	4 3 2	144.44
.7960	24	5 2 1	150.77
.7957	21	4 3 3	150.93
.7933	2	1 1 12	152.32
.7931	3	3 2 9	152.44
.7916	5	3 0 11	153.31
.7884	24	5 2 2	155.36
.7880	5	6 0 4	155.65
.7873	1	5 1 6	156.13
.7844	6	4 2 7	156.23
.7835	7	2 0 12	158.95

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, 4, 5, 6, and 7 [5]

[5] Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.
A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE INDEX—Continued

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

* Natural mineral.

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CUMULATIVE MINERAL INDEX—Continued

*Natural mineral.
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